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4. MODELING FRAMEWORK AND APPROACH

The modeling framework was specifically developed to address each of the objectives of the Housatonic PCB fate and transport modeling effort as described in Section 1.2 and the requirements identified in the development of the conceptual model. In this section, the modeling framework and its significant components are described, including a summary of each of the models selected to represent the Housatonic watershed system, the physical domain of each model, and the manner in which the models will be linked to each other for hydrodynamic, sediment transport, and PCB fate and transport simulations.

4.1 THE MODELING FRAMEWORK

The Supplemental Investigation (WESTON, 2000a) is being performed to gather information for use in determining if remediation of areas contaminated with PCBs in the Lower River is necessary, and if so, where and to what extent. Addressing this complex question and other technical issues requires developing an appropriate modeling framework to serve as one of the primary technical tools for decisionmaking. Such a framework must be able to address both historical and future conditions and questions involving various remediation scenarios, including no action.

Furthermore, a modeling framework is needed because no single model is capable of representing all the physical, chemical, and biological processes that apply to this investigation over the wide range of spatial and temporal scales existing at the site, as illustrated in the previous discussion of the conceptual model for the site.

Figure 4-1 illustrates the basic modeling framework for this investigation, including the specific modeling codes and the purpose for which the code will be used. Within this framework, the watershed model, HSPF, encompasses the largest spatial extent of the system, the Hydrologic Study Area. The principal use of HSPF is to establish external boundary conditions for the models being applied within the Primary Study Area (PSA). The PSA is further modeled by the hydrodynamic/sediment transport model, EFDC, and the PCB bioaccumulation model, AQUATOX. Thus, the EFDC and AQUATOX models are effectively nested within the larger spatial domain of the HSPF model.

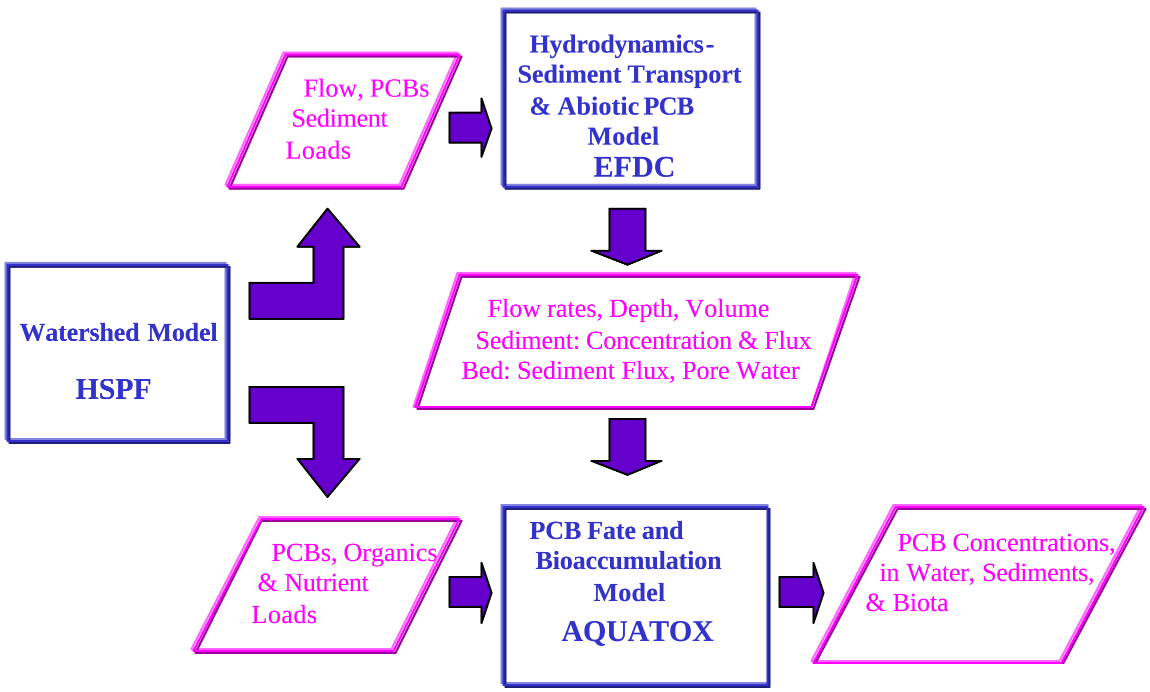


Figure 4-1 Housatonic River PCB Modeling Framework

Logically, the exchange of model outputs as inputs to other models will be aggregated in space and time in a manner consistent with the spatial and temporal scales simulated by each respective model. Thus, the outputs from the watershed model (HSPF) will serve as inputs to the hydrodynamic/sediment transport model (EFDC), and the PCB bioaccumulation model (AQUATOX). For example, surface and subsurface flows, solids, and PCB loading rates simulated by the watershed model will be used to define loading inputs at specific locations within the physical domains defined by EFDC and AQUATOX. Mass fluxes of water and solids (deposition and resuspension, as separate fluxes) simulated by EFDC will subsequently be post-processed as input to AQUATOX at a coarser spatial and temporal resolution, consistent with the coarser segmentation scheme required by this model. A separate abiotic PCB fate and transport component is included in EFDC. The abiotic PCB component is included in EFDC to evaluate the consequences of the spatial and temporal aggregating scheme outlined in this conceptual framework, and to serve as the mechanism to transport PCBs into the floodplain. Model linkage issues are discussed in detail in Section 4.4.

The spatial domain, model time step, and the characteristics of each model are further identified in Table 4-1. The "spatial domain" column in Table 4-1 defines the physical portion of the watershed/river system represented by each model (greater detail, including the scale at which the models are being applied, is provided in Section 4.3); the "time step" column shows the time step of the internal model process calculations. The "constituents" column identifies the key output variables calculated by each model, which are either inputs to the other models, outputs that are compared with field observations as part of the calibration effort, and/or the critical model predictions (e.g., PCB concentrations).

Figure 4-2 shows the Housatonic River watershed upstream of the U.S. Geological Survey (USGS) gaging station (ID # 01197500) at Great Barrington, MA, an area of about 282 square miles. Figure 4-2 also shows the mainstem of the Housatonic River, the major tributaries, subbasin drainage areas, and the PSA represented by the 10-year floodplain (shaded area) between the confluence of the East and West Branch and Woods Pond. An expanded view of the area between Dalton and Woods Pond, including the PSA, is shown in Figure 4-3.

Table 4-1

Housatonic River PCB Modeling System Components

Model	System Component	Spatial Domain	Time Step	Constituents
HSPF	Watershed Hydrology and NPS Loads	Watershed area headwaters to Great Barrington, 282 square miles	Hourly	Flow, solids, PCBs, and nutrient loads
EFDC	Hydrodynamics, Sediment, and Abiotic PCB Transport	Confluence of East and West Branches to Woods Pond Dam	Variable, minutes	Flow, stage, abiotic PCBs and solids (cohesive and noncohesive)
AQUATOX	PCB Fate and Bioaccumulation	Confluence of East and West Branches to Woods Pond Dam	Variable; daily output	PCBs, DO, organic matter, nutrients, solids, detritus, aquatic biota

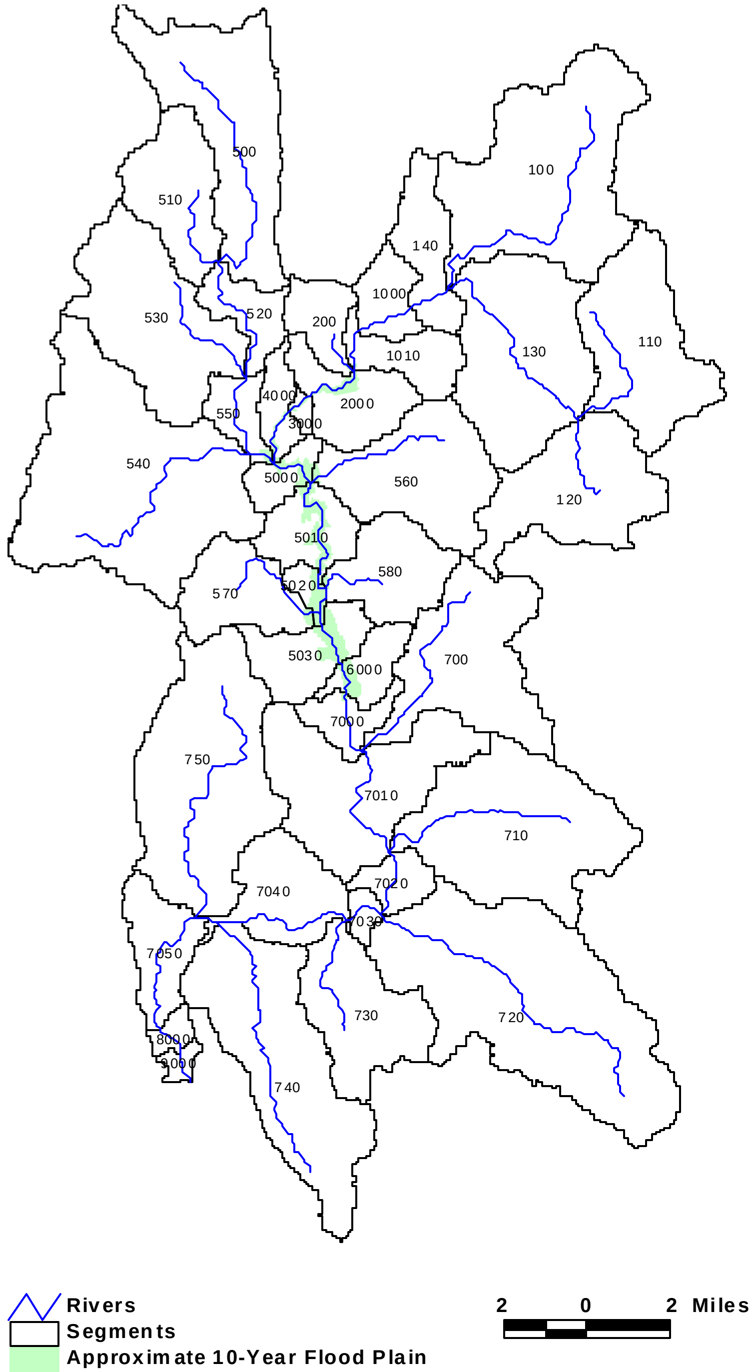


Figure 4-2 Housatonic River Watershed Segmentation

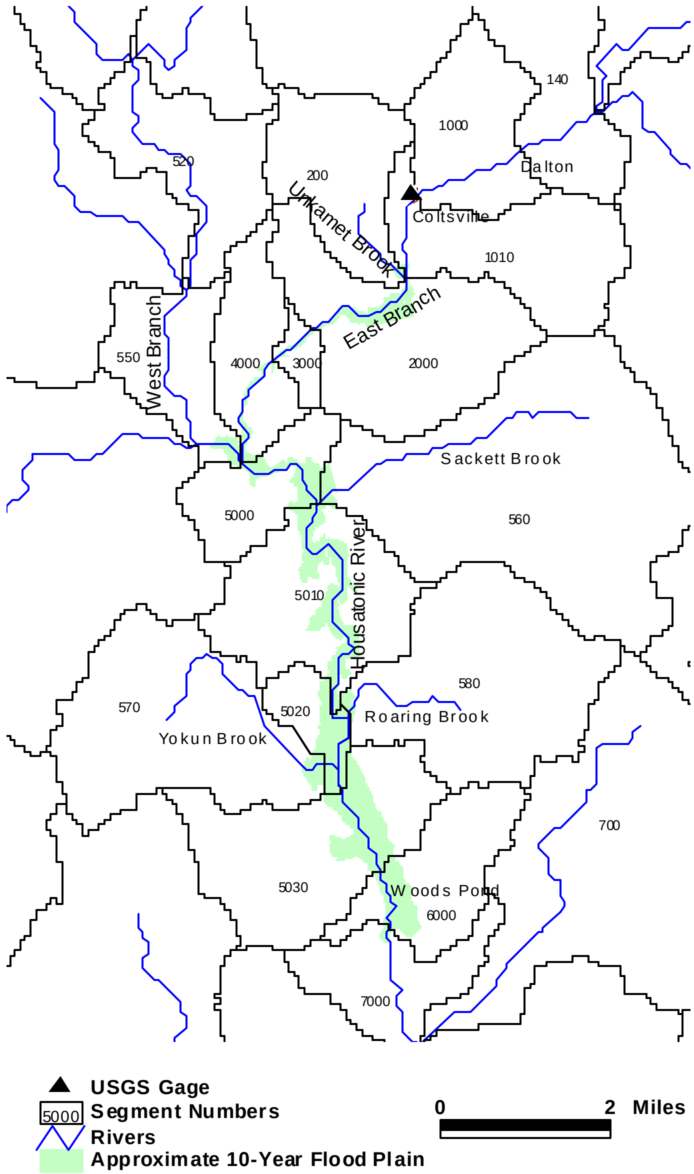


Figure 4-3 Watershed Model Segmentation Within the Primary Study Area

4.2 SUMMARY OF COMPONENT MODELS

The three component models are briefly described in this section, with an expanded discussion and additional source references for each model provided in the appendices (see Appendices B, C, and D).

4.2.1 HSPF

4.2.1.1 Overview

The Hydrological Simulation Program-FORTRAN, known as HSPF, is a mathematical model developed under EPA sponsorship to simulate hydrologic and water quality processes in natural and man-made water systems. It is an analytical tool that has application in the planning, design, and operation of water resource systems. The model enables the use of probabilistic analysis in the fields of hydrology and water quality management. HSPF uses such information as the time history of rainfall, temperature, evaporation, and parameters related to land use patterns, soil characteristics, and agricultural practices to simulate the processes that occur in a watershed.

Runoff flow rate, sediment loads, nutrients, pesticides, contaminants, and other water quality constituent concentrations can be predicted. The model uses these results and stream channel information to simulate instream processes. From this information, HSPF produces a history of water quantity and quality at any point in the watershed.

HSPF is one of the most comprehensive and flexible models of watershed hydrology and water quality currently available. It is one of very few models that can simulate either continuous, dynamic event, or steady-state behavior of both hydrologic/hydraulic and water quality processes in a watershed, with an integrated linkage of surface, soil, and stream processes. The model is also unusual in its ability to represent the hydrologic regimes of a wide variety of streams and rivers with reasonable accuracy. It has been applied to such diverse climatic regimes as the tropical rain forests of the Caribbean, the arid conditions of Saudi Arabia and the southwestern United States, the humid conditions of Europe and the eastern United States, and snow-covered regions of eastern Canada.

Historical Development

HSPF was first released publicly in 1980, as Release No. 5 (Johanson et al., 1980), by the EPA Water Quality Modeling Center (now the Center for Exposure Assessment Modeling). Throughout the 1980s and early 1990s, HSPF underwent a series of enhancements, culminating in the release of Version No. 11 in 1997 (Bicknell et al., 1997). HSPF Version No. 12 (Bicknell et al., 2000) is scheduled for final release in late 2000 with additional software and water quality model algorithm enhancements funded by a variety of federal, state, and regional agencies.

Since 1981, the USGS has supported HSPF development work and has been developing software tools to facilitate watershed modeling by providing interactive capabilities for model input development, data storage and data analysis, and model output analysis including hydrologic calibration assistance. The most recent major product of these efforts is the GenScn GUI interface to HSPF (Kittle et al., 1998) designed to perform these interactive capabilities; GenScn and HSPF Version No. 12 will be applied in this study.

Since its initial release in 1980, HSPF applications have been worldwide and number in the hundreds; more than 50 current active applications continue around the world, with the greatest concentration in North America. Numerous studies have been completed or are continuing in the Pacific Northwest, the Washington, DC, metropolitan area, and the Chesapeake Bay region. Today the model serves as the focus for cooperation and integration of watershed modeling and model support efforts between EPA and USGS. HSPF was recently selected as the key watershed modeling component for the EPA BASINS system (Lahlou et al., 1998), a tool for supporting development of total maximum daily loads (TMDLs) required under Section 303(d) of the Clean Water Act. In addition, HSPF is currently being incorporated into the USACE Watershed Model System (WMS) (Deliman et al., 1999). Over the years, these development activities, model enhancements, and model applications have continued to improve the model's capabilities and preserve its status as a state-of-the-art tool for watershed analysis.

Overview of HSPF Capabilities and Components

HSPF contains three application modules and five utility modules. The three application modules simulate the hydrologic/hydraulic and water quality components of the watershed. The utility modules are used to manipulate and analyze time-series data. Table 4-2 summarizes the constituents and capabilities of the HSPF application modules.

The three application modules within HSPF, and their primary functions, are as follows:

(1) PERLND—Simulates runoff and water quality constituents from pervious land areas in the watershed.

(2) IMPLND—Simulates impervious land area runoff and water quality.

(3) RCHRES—Simulates the movement of runoff water and its associated water quality constituents in stream channels and mixed reservoirs.

A variety of storage zones are used to represent the processes that occur on the land surface and in the soil horizons. Snow accumulation and melt are also included in the PERLND module so that the complete range of physical processes affecting the generation of water and associated water quality constituents can be represented. Some of the many capabilities available in the PERLND module include the simulation of:

- Water budget and runoff components.
- Snow accumulation and melt.
- Sediment production and removal.
- Accumulation and washoff of user-defined nonpoint pollutants.
- Nitrogen and phosphorus fate and runoff.
- Pesticide fate and runoff.
- Movement of a tracer chemical.

IMPLND is used for impervious land surfaces, primarily for urban land categories, where little or no infiltration occurs. However, some land processes do occur, and water, solids, and various pollutants are removed from the land surface by moving laterally downslope to a pervious area, stream channel, or reservoir. IMPLND includes most of the pollutant washoff capabilities of the commonly used urban runoff models, such as the STORM, SWMM, and NPS models.

RCHRES is used to route runoff and water quality constituents simulated by PERLND and IMPLND through stream channel networks and reservoirs. The module simulates the processes

Table 4-2

HSPF Application Modules and Capabilities

PERLND	IMPLND	RCHRES
Snow	Snow	Hydraulics
Water	Water	Conservative Constituents
Sediment	Solids	Temperature
Soil temperature	Water Quality*	Sediment
Water Quality*		Nonconservative Constituents
Pesticide		BOD/DO
Nitrogen		Nitrogen
Phosphorus		Phosphorus
Tracer		Carbon/pH
		Plankton

*Up to 10 user-specified water quality parameters.

that occur in a series of open or closed channel reaches or a completely mixed lake. Flow is modeled as unidirectional. A number of processes and parameters can be modeled, including:

- Hydraulic behavior.
- Heat balance processes that determine water temperature.
- Inorganic sediment deposition, scour, and transport by particle size.
- Chemical partitioning, hydrolysis, volatilization, oxidation, biodegradation, and generalized first-order (e.g., radionuclides) decay, parent chemical/metabolite transformations.
- DO and BOD balances.
- Inorganic nitrogen and phosphorus balances.
- Plankton populations.
- pH, carbon dioxide, total inorganic carbon, and alkalinity.

4.2.1.2 HSPF Data Requirements

Data requirements for HSPF are extensive, in both spatial and temporal detail, especially for a watershed of the size and complexity of the Housatonic. Table 4-3 lists the typical data requirements for running an HSPF application on a river such as the Housatonic. Fortunately, for this study an extensive database exists to support such an application. As noted in Section 3, historical data collected by GE, EPA, USGS, and various state agencies, supplemented by the ongoing data collection efforts of these same groups, provides a sound basis for the watershed modeling effort.

Precipitation and Meteorologic Data

Precipitation is the primary driving force in any watershed modeling effort, followed in importance by evaporation and air temperature; the remaining meteorologic data (listed in Table 4-3) are required for modeling snow accumulation and melt processes, and water temperature. In Appendix F, Table F-8 shows the available precipitation and meteorologic data within and neighboring the Housatonic River watershed. Long-term hourly precipitation data required to drive the watershed modeling effort is limited to the National Weather Service (NWS) station at

Table 4-3

Data Requirements For Typical HSPF Model Applications

1.	**Precipitation and meteorologic data (for simulation period)**	
	a.	Hourly Precipitation
	b.	Daily pan evaporation
	c.	Daily maximum and minimum air temperature
	d.	Total daily wind movement
	e.	Total daily solar radiation
	f.	Daily dewpoint temperature
	g.	Average daily cloud cover
2.	**Watershed land use/land cover characteristics**	
	a.	Topographic map/data of watershed and subwatersheds
	b.	Land use/cropping delineation and acreages
	c.	Soils delineation and characteristics
3.	**Hydrography and channel characterization**	
	a.	Channel lengths and slopes
	b.	Channel cross sections and geometry
	c.	Channel bed composition
	d.	Diversions, point sources, channelization segments, etc.
	e.	Tributary area (and land use distribution) for each channel reach
4.	**Monitoring program observations**	
	a.	Flow rates during all monitored storm events
	b.	Flow volume/rate totals for storm/daily, monthly, annual
	c.	Sediment concentrations and mass losses in runoff
	d.	Chemical concentrations and mass losses in runoff
	e.	Soil concentrations of chemical/nutrient forms, if available
	f.	Estimated/actual chemical concentrations in precipitation
	g.	Particle size distributions (sand, silt, clay fractions) of soils and eroded sediments
5.	**Other useful information**	
	a.	Description/quantification of any other contaminant sources (e.g., point sources) or other relevant information (e.g., ponds, dams, marshes)
	b.	Technical reports or articles that analyze and/or summarize the monitoring data
	c.	Soils characterization information for estimating model parameters

Lanesborough, MA (in model segment #500, shown in Figure 3-2) in the northern portion of the watershed, and the NWS stations at Littleville Lake, MA (about 20 miles east) and Copake, NY (about 20 miles southwest). In addition, since 1994, GE has collected 15-minute and hourly data at its Pittsfield facility; these GE data will be used extensively for the most recent time period because it is the closest location to the PSA.

There are a number of currently active NWS stations with long-term daily precipitation data surrounding the watershed, e.g. Great Barrington Airport, West Otis, Chesterfield, and Berlin (see Table F-8). The standard practice in watershed modeling is to use the available hourly data to distribute (or disaggregate) the daily records to derive estimated hourly records (and distribution during the day) at these stations. Thus, the hourly data at Lanesborough and the GE facility, supplemented by the Littleville Lake and Copake stations (as needed), will be used to distribute these daily records into hourly values for use in neighboring portions of the watershed.

Pan evaporation data are used in watershed modeling to estimate total potential evapotranspiration (PET), which includes both direct evaporation and plant transpiration processes. Typically a "pan coefficient" is applied to the observed pan evaporation data, either on an annual or monthly basis, to estimate PET; pan coefficients have been tabulated and mapped for the conterminous U.S. by the National Weather Service (NWS, 1982a; 1982b). For the Housatonic River watershed, the closest pan evaporation data are recorded at the Albany and Hartford airports, which are approximately 30 miles northwest and southeast, respectively, from the watershed (see Figure 1-1). Pan evaporation does not demonstrate much spatial variability, and it is common practice to use pan evaporation data from such distances for watershed modeling. The Albany and Hartford data will be supplemented and compared with recent pan evaporation data collected by GE at its Pittsfield, MA, facility starting from 1999.

Daily maximum and minimum air temperature readings are collected at many of the same NWS stations that collect daily precipitation; thus many of these same stations are listed in appendix Table F-8 for air temperature. The hourly temperature data collected at the GE facility will be used for the time period starting in 1994 with the daily data used for the earlier time periods. The daily values are distributed to hourly by imposing a standard sinusoidal variation during the day. Since hourly values are available at the GE facility, the standard sinusoidal distribution will be checked with the GE data and adjusted as needed. In addition, air temperature values are adjusted as a function of elevation differences between the gage site and the model segment.

For the remaining meteorologic data, i.e., solar radiation, wind, dewpoint temperature, and cloud cover, observations at either Albany or Hartford will be used and supplemented with the available GE Pittsfield data. Periods of missing data are typical of all meteorologic data; the additional stations listed in Appendix F will be used to supplement those mentioned above and fill in any missing periods.

Watershed Land Use/Land Cover Characteristics

The watershed land use and land cover data were discussed in Section 4.3.1 as part of the watershed segmentation and characterization of the physical domain of the watershed model. Based on the DEM data and procedures described in that section, Appendix D provides lists of the segment areas, land uses and associated areas within each segment, and slopes for each model segment. In addition, major soil types and characteristics, such as texture, erodibility, bulk density, available water capacity, and hydraulic conductivity, can be identified and tabulated for each model segment as a basis for parameterization.

Hydrography and Channel Characterization

Section 4.3.1 describes the model domains and identifies the procedures used to estimate the major channel characteristics within each model segment; Appendix D lists the estimated channel lengths, slopes, and elevation changes within each reach. This information will be supplemented with cross-section data collected by EPA and GE, USGS rating curves (i.e., stage versus discharge curves) for their gages within the watershed, the GE 1997 bathymetric survey and bed sediment mapping data (QEA, 1998a, 1998b), and additional cross-section data needed for the EFDC grid development. Within the channel module of HSPF, each stream reach is represented by a hydraulic function table, called an FTABLE, that defines the flow rate, surface area, and volume as a function of the water depth. Since HSPF uses a much simpler representation of channel processes than EFDC, the data required for EFDC (discussed in Section 4.6.2) are entirely adequate for the channel simulation data needs within HSPF. The data currently developed and listed in Appendix D are considered “preliminary” because the reach boundaries will be modified to coincide with specific EFDC grid cells and AQUATOX segments when the spatial representation for both models is finalized.

HSPF Data Requirements

The HSPF watershed model calibration will rely on available data at the USGS Coltsville and Great Barrington gages, supplemented with the synoptic and stormwater monitoring data collection, both past and current, performed by Roy F. Weston, Inc., as part of the SIWP, and by GE. Observed data are required for all the constituents simulated by HSPF in this effort, including flow, sediment, water temperature, DO, BOD, TOC, nutrients, and PCBs.

The hydrology calibration will focus primarily on the available continuous flow data at the two USGS gages, and will perform consistency checks with synoptic flow measurements available for selected tributaries and other monitoring sites within the PSA. Although Table 3-1 shows the recent sediment and water quality data covering a period of years since 1994 and 1995, the data are not continuous. Consequently the watershed water quality calibration will rely on comparisons of observed and simulated concentrations at selected sites and selected points in time, covering a limited number of both storm and nonstorm periods. The ongoing SIWP stormwater sampling is designed to supplement the available historical data. However, these comparisons will be made within the overall mass balance approach and framework discussed in Section 1.3 to ensure that a reasonable mass balance for flow, solids, and PCBs is represented within the watershed model. Further discussion of the details of calibration and validation of HSPF is presented in Section 4.5 of the Modeling Study QAPP (Beach et al., 2000).

Initial Conditions

Evaluation of initial conditions is less critical for the HSPF watershed model than for the EFDC and AQUATOX models because the watershed is a self-contained, well-defined system not impacted by external forces at its spatial boundaries (i.e., drainage basin). The driving forces are meteorologic conditions, represented by the time series of precipitation, evaporation, and other climate inputs, along with any anthropogenic inputs (e.g., point-source loads) and impacts. To avoid any short-term effects of initial starting values of state variables (e.g., soil moisture conditions), the model is usually run for many years, and starting conditions are then readjusted to reflect state variable conditions at comparable times during subsequent years of the model run. For example, if the model run starts on 1 October, soil moisture conditions at the beginning of October for subsequent years will be evaluated as a basis for readjusting the starting moisture conditions of the run. Climate conditions prior to the model run will also be checked to assess whether further adjustments are needed. In most cases, starting values will only impact model simulations for a short time period (e.g., a few weeks to a few months), and often simulations are begun 6 months to a year before the period of interest to avoid any potential impacts of the starting condition values.

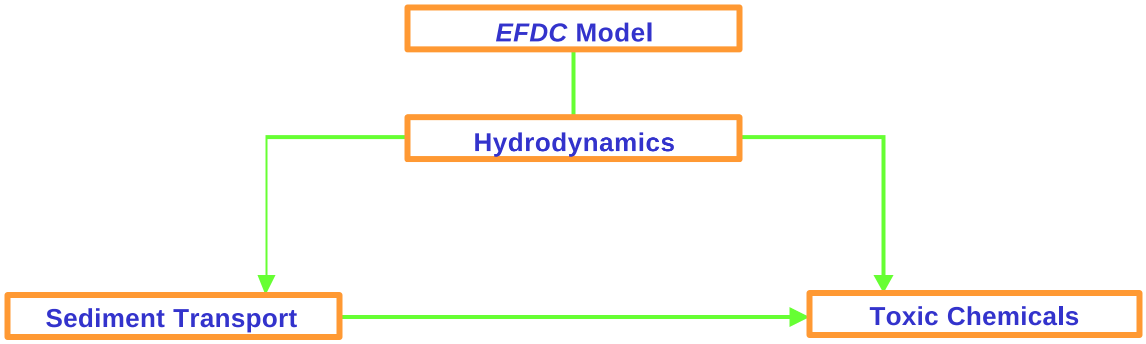
4.2.2 EFDC

4.2.2.1 Overview

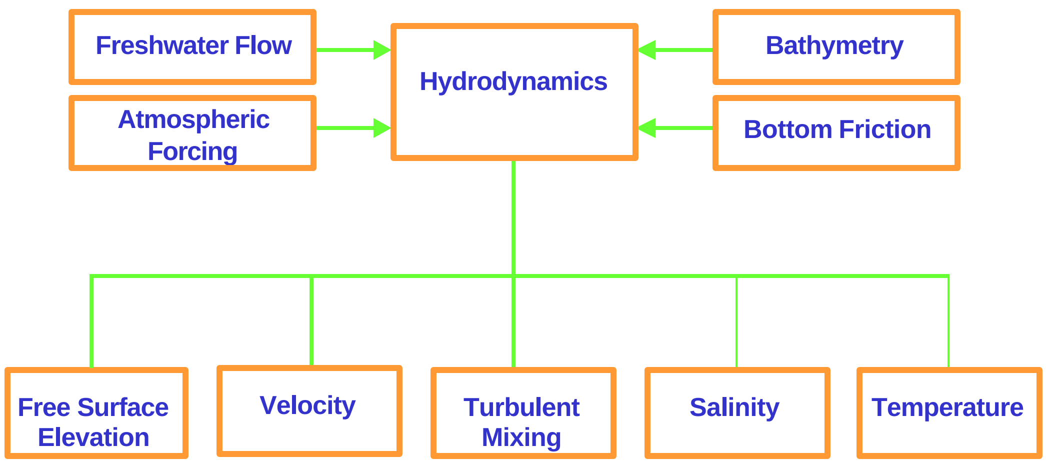
The Environmental Fluid Dynamics Code (EFDC), a public domain model sponsored by the Commonwealth of Virginia and EPA, is a 3-D computational physics model that incorporates modules for hydrodynamics, sediment transport, contaminants, and eutrophication/water quality within a single source code (Hamrick, 1992a; 1992b). Figures 4-4 and 4-5 present schematic diagrams of the conceptual linkage in EFDC between the hydrodynamic, sediment transport, and contaminant submodels that will be applied in the Housatonic River study.

EFDC uses a finite difference spatial grid scheme to represent the physical domain of a waterbody as a fully 3-D domain; lateral or vertical averaging is used to represent a waterbody in either one-dimensional (1-D) or two-dimensional (2-D) domains. The physical domain is represented in the vertical domain using a stretched (“sigma”) coordinate scheme and in the horizontal domain the waterbody is represented with either (a) cartesian; (b) boundary fitted, curvilinear-orthogonal grid schemes, or c) some combination of the two.

EFDC can be executed in two modes: (1) fully coupled mode with simultaneous computation of hydrodynamics, sediment and contaminant transport and fate, or (2) hydrodynamic transport-

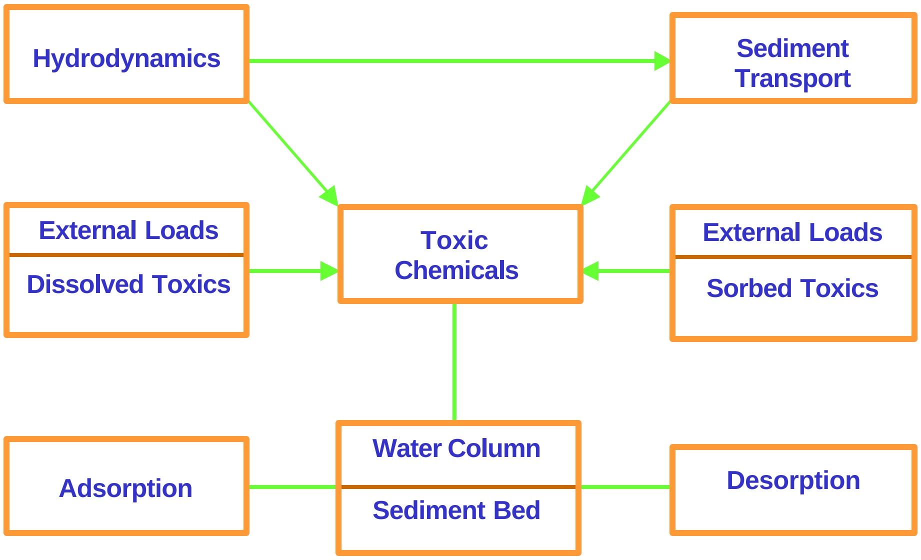


Primary Sub-Models of the EFDC Model

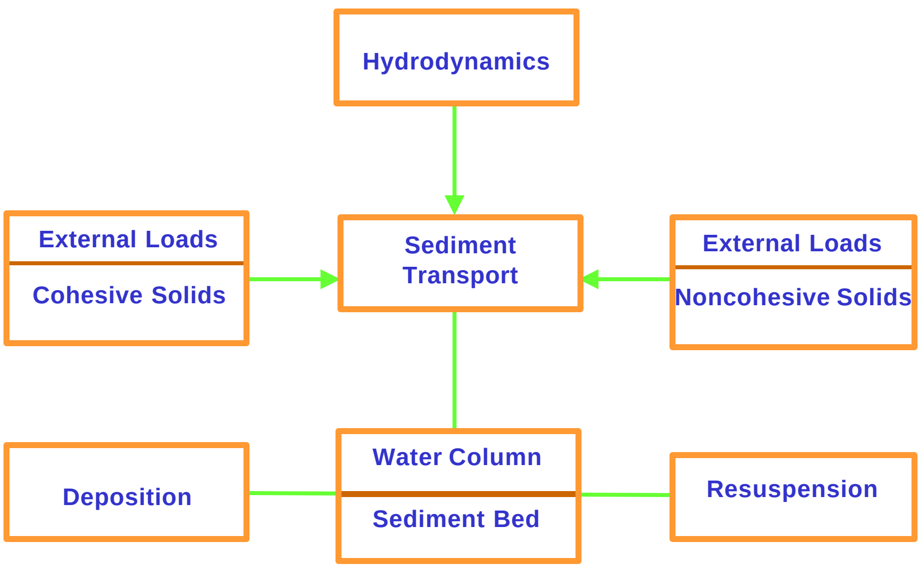


Structure of the EFDC Hydrodynamic Model

Figure 4-4 Structure and Modules of the EFDC



Model Structure of the EFDC Sediment Transport Model



Structure of the EFDC Toxic Model for Abiotic PCBs

Figure 4-5 Structure of EFDC Sediment Transport Model and Toxic Model for Abiotic PCBs

only mode with the distribution of sediments and chemical constituents simulated by using saved hydrodynamic data as an external input file to drive the constituent transport and fate submodels. The computational techniques used in EFDC have been shown to be very efficient (Hamrick and Wu, 1997) in benchmark tests of internal processing speed where EFDC executed about a factor of two faster (Wu et al., 1997c) than the well-known ECOM3D model (Blumberg and Mellor, 1987).

EFDC has been extensively tested and applied for many modeling studies of hydrodynamics, sediment transport, contaminants, and eutrophication in complex marine (e.g., Chesapeake Bay, Hamrick, 1994a) and freshwater (e.g., Florida Everglades, Hamrick, 1994b) ecosystems.

EFDC has been applied in estuarine cohesive sediment transport simulations (Yang, 1996; Tetra Tech, 1999c) and coastal noncohesive sediment transport (Zarillo and Surak, 1995). The model is currently being applied to investigate cohesive sediment transport in Lake Okeechobee, FL (Hamrick, 1996b). EFDC has been applied for simulations of solids and metals transport and fate in the Blackstone River (Tetra Tech, 1999a) and solids, metals, and organic contaminants transport and fate in the Duwamish Waterway-Elliott Bay in Puget Sound (Tetra Tech, 1998).

An overview of the key processes of the hydrodynamic, sediment transport, and contaminant submodels of EFDC is presented below. The features of EFDC used for the Housatonic River study are described in Appendix C.1. The theory and formulations incorporated in the sediment transport model (Tetra Tech, 2000d) are described in Appendix C.3. Complete descriptions of the options available in EFDC are presented in the user's manual (Hamrick, 1996a). Technical details of the theory and model formulations for the hydrodynamic model are found in Hamrick (1992a). The model formulations in EFDC for the toxic contaminant submodel are detailed in Tetra Tech (1999e).

Hydrodynamics

The hydrodynamic component of EFDC simulates the 3-D equations of motion based on conservation of mass and momentum to compute velocity and turbulent mixing in the horizontal and vertical domains. The physics of the EFDC model, as well as many features of the computational schemes, are functionally equivalent to the well-known Blumberg and Mellor (1987) model of hydrodynamics. Designed for application to marine or freshwater systems, EFDC solves the 3-D vertically hydrostatic, free surface, turbulent averaged, coupled barotropic, and baroclinic equations of motion for a variable density field. Dynamically coupled transport equations for turbulent kinetic energy and turbulent length scale, solved using two turbulence parameter transport equations, are based on Galperin's et al. (1988) modification of the Mellor and Yamada (1982) level 2.5 turbulence closure scheme. These formulations are used to simulate eddy viscosity and diffusivity in the vertical direction. The bottom stress formulation for friction, describing the rate of momentum loss at the sediment bed-water interface, is represented using a turbulent boundary layer formulation via a quadratic function of near-bottom velocity.

Salinity and water temperature are solved as an integral part of the hydrodynamic model with heat transport simulated using the atmospheric heat exchange model developed by Rosati and Miyakoda (1988) at the NOAA Geophysical Fluid Dynamics Laboratory. Enhancements to EFDC have been designed to allow for specification of (a) wetting and drying of shallow areas using a mass-conserving scheme for applications for wetlands, tidal flats, or floodplains and (b) discharge control structures such as weirs, dam spillways, and culverts. For the simulation of flow in heavily vegetated areas, such as wetlands or riverine floodplains, EFDC uses a formulation developed for the Florida Everglades (Hamrick, 1994b) to represent vegetation friction resistance.

The dominant physical factors that will influence hydrodynamic transport in the Housatonic River are changes in topographic elevation of the riverbed (i.e., channel slope), bottom friction from the sediment bed, the extreme sinuosity of numerous meanders within a wide floodplain, and the presence of backwaters and a broad impoundment created by the Woods Pond Dam.

The computational burden for an EFDC riverine application to an area of the scope and nature of the Housatonic River is anticipated to be quite large. Work is being conducted to investigate code enhancements and model constructs to improve model computational efficiency. Areas being investigated are parallel processing, coding optimizations/streamlining, variable timestepping schemes, and stepped hydrodynamics. Changes to the code will undergo thorough third-party review and testing and will become part of the calibration report.

Sediment Transport

The sediment transport module of EFDC allows for specification of multiple size classes to describe both cohesive and noncohesive solids. The transport of solids suspended in the water column is based on the same advection and diffusion scheme that is used for heat transport (i.e., water temperature) and salinity in the hydrodynamic model. The transport of solids in the sediment bed (bedload) by sliding, rolling, or saltation on, or near, the bed is based on near-bottom velocity and the particle size and density characteristics. The transport of solids in the river is thus governed by the external supply of solids washed from the watershed and the internal supply of solids from the sediment bed.

Solid particles in natural waters, described using characteristic size fractions as (a) cohesive silts and clays (less than 63 microns) and (b) coarser noncohesive materials (63 to 250 microns, and greater than 250 microns), settle out of the water column as a result of gravitational force. Depending on the force of the ambient flow conditions, particles can also be eroded from the sediment bed and resuspended into the water column. At low solids concentrations, the settling velocity for noncohesive solids is primarily dependent on the discrete particle size. Under high solids concentrations, the settling velocity of noncohesive materials can be reduced by hindered settling conditions near the riverbed (van Rijn, 1984; Cao et al., 1996).

At the water column-sediment interface, the net vertical flux of noncohesive solids is controlled primarily by the shear stress of near-bottom flow and the particle size and density of the noncohesive materials in the surficial sediments. Under equilibrium conditions for flow and solids loading, the water column equilibrium concentration of noncohesive solids can be functionally described using particle size and density, bed stress, and vertical turbulent diffusivity (Garcia and Parker, 1991; Smith and MacLean, 1977; Van Rijn, 1984). Under nonequilibrium conditions, the net flux of noncohesive sediment between the bed and the water column is dependent on the near-bed settling velocity and the gradient between the equilibrium and actual near-bed concentration.

The settling behavior of cohesive particles is quite complex since individual cohesive particles may flocculate into larger clumps of material that have very different settling characteristics than the individual particles that make up the floc. As an alternative to computationally intensive "first principle" models that are under development for describing settling of cohesive particles, the settling velocity of flocs has been parameterized into empirical functional relationships (Ariathurai and Krone, 1976; Hwang and Mehta, 1989; Ziegler and Nisbet, 1994; Shrestha and Orlob, 1996) in terms of fundamental particle size, cohesive solids concentration, and shear characteristics of the turbulent flow regime.

Net deposition of cohesive materials between the water column and sediment bed is related to the flow-induced bed surface stress and the properties of the cohesive material. As bed stress decreases in relation to a critical shear stress for deposition of cohesive particles, the probability of particle deposition tends to increase. Resuspension of cohesive solids from the bed into the water column occurs by (a) mass and (b) surface erosion modes. Mass erosion occurs rapidly when the flow-induced bed shear stress exceeds the depth-dependent shear strength of the sediment bed. Surface erosion, in contrast, occurs slowly when the bed stress is less than the bed shear strength near the surface but greater than a critical resuspension stress dependent on the shear strength and density of the bed.

The sediment bed may be represented in EFDC with either a single-surface sediment layer or multiple sediment layers. The multiple-layer sediment bed is represented by a user-specified maximum number of layers having time-varying thicknesses and porosity or void ratio. The void ratios of the multiple layers are either (a) specified as input by the user or (b) determined internally by an empirical relationship or dynamic bed-consolidation model. Vertical transport of sediment and sorbed contaminants (such as PCBs) between bed layers is implicitly represented by sediment particle displacement in response to layer thickness variations dynamically determined by the bed consolidation formulation. The multiple-layer bed enables a relationship of time-since-deposition as a function of the depth in the sediment bed to be established. Changes in the water column-sediment bed interface elevation can also be incorporated as an option in the hydrodynamic model to provide bathymetric feedback to the continuity equation.

Contaminants

With many contaminants (such as PCBs) exhibiting preferential partitioning onto solids, the chemical submodel of EFDC is designed to be coupled with the sediment transport submodel, with the contaminants represented as abiotic constituents. The chemical submodel enables the mass balance simulation of contaminants in both the water (dissolved) and sediment (particulate) phases of the water column and the sediment bed. Water-sediment phase interactions are represented by either equilibrium partitioning or nonlinear sorption processes. With the sediment bed described by multiple layers, sediment bed water volume and dissolved contaminant mass balances allow contaminants to be transported back into the water column by sediment resuspension, pore water expulsion due to bed consolidation, and pore water diffusion.

4.2.2.2 EFDC Data Requirements

The modules of the EFDC model that will be used for the Housatonic River study include the hydrodynamic, sediment transport, and abiotic PCB transport and fate submodels.

The hydrodynamic model requires physical information to describe grid cell geometry, inflows and outflows of water, bottom friction and elevations of the water surface and the riverbed, and other physical forcings (e.g., hydraulic control structures) that influence the transport of water in a riverine environment. The sediment transport model requires data to describe the spatially and temporally varying cohesive and noncohesive sediment distributions in the riverbed and the water column.

The sediment transport model requires specification of the cohesive and noncohesive sediment characteristics of solids loading from point and nonpoint sources to the river. Information is also needed to parameterize the depositional and erosional characteristics of cohesive and noncohesive sediments to simulate the vertical transport of solids between the water column and the riverbed.

The abiotic PCB model requires data to describe the spatially and temporally varying distributions of PCBs in the riverbed and the water column. The abiotic PCB model, representing both dissolved and sorbed contaminants, requires data to define the transfer of PCBs between the dissolved and particulate phases via equilibrium partitioning, and transfer between the water and atmosphere via volatilization if implemented.

Hydrodynamic Model

EFDC requires the following physical input data for the hydrodynamic simulation:

Horizontal Grid Specification

- **Grid Cell Geometry—**Water surface elevation, riverbed and floodplain elevations, and initial conditions of water depth, volume, length, and width are specified for each EFDC grid cell in the physical domain of the Housatonic River study area. Physical data will be obtained from cross-section surveys of (a) numerous transects taken along the Housatonic River in the vicinity of Pittsfield, MA, upstream of the confluence, (b) transects taken to characterize topography and channel depths for the meanders, backwaters, floodplain, and Woods Pond, and (c) the data provided by GE from its 1997 monitoring and bathymetric/bed sediment survey (QEA, 1998a, 1998b).

Bathymetric data are needed to define the spatial variation of water column depth in Woods Pond and the backwater areas upstream of Woods Pond. Very detailed bathymetric data for Woods Pond and the backwater areas are available from a survey conducted for this study in December 1998. The survey data from December 1998 will be used to characterize the spatial distribution of depth in Woods Pond and the backwater areas for the EFDC simulation of "contemporary" conditions circa 1998-1999. Comparable detailed bathymetric data for Woods Pond and the backwaters are not available for the representation of historical conditions circa early 1980s.

The net sediment accumulation rate in Woods Pond has been estimated based on sediment core measurements of cesium-137, lead-210, and beryllium-7. Using detailed bathymetry data and sediment thickness measured in 1998 in combination with estimates of the net sediment accumulation rate extrapolated over a period of ~20 years, estimates of the bottom depths of Woods Pond will be developed to represent bathymetry for the simulation of historical conditions circa early 1980s. For the simulation of projected PCB distributions under various remediation alternatives, the 1998 bathymetric data set will be used to define the initial conditions of bottom depth of Woods Pond and the backwater areas. Over the decadal time scale that will be used for remediation scenarios, the bottom depths of Woods Pond and the backwater areas will progressively change as a simulated response to continued net sediment accumulation in the pond.

- **Grid Cell Connectivity**—The horizontal connectivity of each EFDC grid cell is defined by identification of one of the following types of cells represented in the physical domain: water cell; "wetting and drying" cell; land cell adjacent to water cell; or dry land cell. Grid cell types will be identified by overlaying the EFDC discretization grid scheme with GIS files to define EFDC grid cells types as 10-year floodplain, the main river channel, the backwater areas, and Woods Pond.

Initialization Data

- **Initial Conditions—**The initial spatial distributions of water surface elevations and chlorides must be defined to start the simulation. Data to define initial surface water elevations will be obtained from stage height versus streamflow rating curves developed for various reaches of the river. Data to define the initial salt distribution will be obtained from available water quality monitoring records to characterize chloride distributions in the Housatonic River.

Forcing Functions and Boundary Conditions

- **Forcing Functions and Boundary Conditions—**Time series (uniform or non-uniform) are defined to describe the temporal variability of: (a) meteorologic and climatologic data (incident solar radiation, air temperature, precipitation, evapotranspiration, winds); (b) water surface elevation; (c) freshwater inflows and outflows; and (d) concentration of chlorides. The same time series of meteorological and climatological data sets that are used as input to the HSPF watershed model will also be used as input to EFDC to simulate water temperature. Time series of freshwater inflow and chlorides will be provided by linking the output from the coarse HSPF transport reaches as input to the finer spatial resolution of EFDC grid cells. HSPF will provide water inflow to EFDC as time series of surface runoff and subsurface inflows based on simulation results generated for each coarse HSPF transport reach. Both surface and subsurface inflow data will be normalized by the length scale of the long HSPF reaches for input as a unit inflow rate ($m^3s^{-1}m^{-1}$) to the much shorter length of the EFDC grid cells.

Physical Processes

- **Vegetation Resistance—**The frictional influence of vegetation will be represented by parameterization of empirical relationships describing natural flow in heavily vegetated waterways (Hamrick, 1994b). This feature will be used to characterize overland flow within grid cells defined for the 10-year floodplain. Existing wetland delineation, vegetation surveys, and aerial photographs of the floodplain will be used to estimate appropriate vegetative parameter values assigned to floodplain grid cells to distinguish between differing vegetation types.

- **Soil Moisture Model—**A simple soil moisture model, typically used for wetland simulations (Hamrick, 1994b), can be used to describe the temporal and spatial variation of soil moisture within an active zone below each “wetting and drying” grid cell. The effective porosity of the soil layer and a maximum infiltration rate are the key parameters needed to describe the amount of water that can be stored within the soil layer. This feature may be needed to represent the water balance within the “wetting and drying” grid cells of the 10-year floodplain.

- **Hydraulic Control Structures—**Flow between upstream and downstream pairs of grid cells can be controlled by hydraulic structures such as dams, weirs, or spillways and pumping stations. This feature of EFDC will be used in the Housatonic River model to define streamflow over the Woods Pond Dam at the downstream boundary of the physical domain. A rating curve for the dam will be developed to describe streamflow over the Woods Pond Dam spillway as a function of the water surface elevation (stage height) at the dam using the specifications that were established at the time of construction of the dam.

Sediment Transport Model

EFDC requires the following input information for sediment transport simulations. Solids will be defined in the Housatonic River model using three particle size classes to represent cohesive (< 63 microns) and two classes of noncohesive (63-250 microns; > 250 microns) solids.

- **Water Column Initial Conditions—**Initial concentrations for each cohesive and noncohesive solids class are assigned to each model grid cell. This information will be obtained from particle size distributions and water column TSS monitoring samples. Grain size distribution data will be used to estimate the fraction of total solids that is assigned to the cohesive and noncohesive size classes along the length of the river.

- **Sediment Bed Conditions—**The riverbed will be characterized by multiple sediment layers consisting of a surficial “active” layer and one or more “deep” sediment layers. The vertical thickness, bulk density, and solids class distributions for each riverbed layer for each horizontal grid cell is required for each size class of particles. This information will be determined from sediment core data taken at numerous station locations in the river. EFDC will internally compute the corresponding void ratios and bulk densities.

  In situ field data are being collected for this project to characterize bulk density, water content, mean particle size, organic carbon content, critical shear stresses, and erosion rates for a number of locations along the Housatonic River. Since a first-principles model is not available to describe solids deposition and resuspension, a number of empirical models have been developed to represent these processes. Empirical model parameter values determined from field data are thus essential to develop a credible model of cohesive and noncohesive solids transport in the Housatonic River.

Depth-dependent erosion rates and critical shear stress measurements needed for input to EFDC will be obtained using a device called a Sedflume initially developed and tested by McNeil et al. (1996), and a Particle Entrainment Simulator (PES) (Tsai and Lick, 1986). In contrast to data obtained from field measurements of the resuspension potential measured using "shaker" (PES) tests where shear stresses are limited to less than 10 dynes cm^{-2}, the experimental approach of McNeil et al. is designed to provide a characterization of depth-dependent erosion rates and critical stresses for sediment cores ~2 meters thick over a wide range of bottom shear stresses (~1-100 dynes cm^{-2}) that are characteristic of ambient conditions in rivers and lakes. The results of the Sedflume experiments and the PES tests will be used to define the depth-dependent critical stresses that result in resuspension of discrete particles and mass erosion of bottom sediments.

- **Solids Loads—**Time series of inflowing suspended solids loads and concentrations corresponding to point and nonpoint source inflows from surface runoff, tributaries, and wastewater treatment dischargers are required to define external inputs of cohesive and noncohesive solids. The time series of total suspended solids loading that is generated by HSPF will be split to represent the proportion of total solids loading assigned to the cohesive and noncohesive size classes for input to EFDC. Observed grain size distribution data obtained from TSS samples with corresponding streamflow measurements taken from the mainstem of the Housatonic River and selected tributaries will be used to estimate flow-dependent fractional splits of TSS as cohesive and noncohesive solids.

- **Noncohesive Sediment Processes—**Representative particle diameter, density, specific volume, specific gravity, and a reference settling velocity will be assigned to the noncohesive solids class. User-specified critical shear stress, derived from experiments performed on site sediments, will control particle deposition and resuspension processes. EFDC internally computes an equilibrium concentration of noncohesive sediment for simulation of a net flux of particle deposition and resuspension that accounts for hindered settling under high solid concentrations near the riverbed. A constant bed porosity is assigned that is also used to represent the porosity of noncohesive solids being deposited in the riverbed.

  In the riverbed, a maximum concentration (as mass per total volume) of noncohesive solids is assigned for the bed consolidation model. Riverbed armoring by noncohesive solids can be represented in the model using formulations described by Garcia and Parker (1991), van Rijn (1984), and Smith and MacLean (1977). It is expected that the van Rijn formulation will be used if armoring is included in the model. For the single class of noncohesive solids that will be represented, EFDC restricts the thickness of the surface bed equal to the dimensional reference height defined by the user as a multiple of the grain size diameter assigned to noncohesive solids.

- **Cohesive Sediment Processes—**Representative solids density, specific volume and specific gravity, and a reference settling velocity will be assigned to the cohesive size class of solids. A user-specified, or selected, relationship between settling velocity, cohesive solids concentration, and ambient shear or turbulent intensity is used in EFDC to describe the net flux of deposition and resuspension. A user-specified, or selected, relationship between shear strength, surface erosion rates, and surface erosion critical stresses and bed bulk density is used to simulate resuspension processes. User-specified critical boundary stresses are defined for deposition and resuspension. Surface erosion is represented with user-specified data to describe the reference rate for surface erosion and the boundary stress above which surface erosion occurs. Bulk sediment properties, erosion rates, and critical boundary stresses will be obtained from the site-specific field measurements. For the empirical bed consolidation model, the ultimate void ratio and the consolidation time scale must be specified. For the dynamic bed consolidation model, functional relationships between bed compressibility, hydraulic conductivity, and void ratio must be provided as input to the model. Maximum and minimum fluid mud concentrations of cohesive solids are assigned for the bed representation. The void ratio of cohesive solids deposited to the bed is assigned as is a minimum bed void ratio for cohesive solids.

Abiotic PCBs Transport and Fate Model

PCBs will be modeled in EFDC as total PCBs. The transport and fate of PCBs in EFDC will be represented only by abiotic processes. Dissolved and particulate phases of PCBs will be transported via advection and turbulent mixing. PCB fate will be described by equilibrium partitioning for sorption and desorption between contaminants and solids, settling and resuspension of sorbed PCBs, potentially volatilization between the water surface and the atmosphere, and kinetic degradation. Biotic processes that influence the distribution and fate of PCBs will be represented in AQUATOX with mass loading of PCBs provided by HSPF and mass fluxes of water and solids provided by EFDC as external loads. EFDC requires the following input data for PCB transport and fate simulations:

- **Water Column Initial Conditions—**Initial total PCB concentrations in the water column will be assigned to each model grid cell. Partition coefficients assigned to the noncohesive and cohesive solids classes will be used internally in the model to compute the dissolved and solid phases of PCBs.

- **Sediment Bed Initial Conditions—**The riverbed will be characterized by multiple sediment layers consisting of a surficial “active” layer and one or more “deep” sediment layers. Total PCB concentration for each riverbed layer and each horizontal grid cell is required. This information will be determined from depth-dependent PCB measurements taken from sediment core data. EFDC will internally compute the corresponding dissolved and particulate phases of PCBs from partition coefficients.

- **PCB Loads—**Time series of PCB loading rates corresponding to point and nonpoint source inputs from surface runoff, groundwater-influenced flux, tributaries, municipal and industrial wastewater treatment dischargers, and atmospheric deposition (wet and dry) are required to define external inputs of the PCBs to EFDC. The time series of surface runoff of PCB loads generated for each coarse HSPF transport reach will be used with estimates of the dissolved and particulate fractional splits to define the input data needed for the finer resolution EFDC grid cells. The time series of subsurface discharge rates simulated in HSPF for assignment to each EFDC grid cell will be coupled with estimates of the pore water PCB concentrations to generate the loading rates of dissolved PCBs from subsurface inflows to the river. For the long-term simulation projections of remediation scenarios, spatial and temporal distributions of pore water PCB concentrations will be defined to reflect each remediation scenario.

- **Abiotic Processes—**Equilibrium partitioning coefficients will be assigned for the two noncohesive and cohesive solids classes. Separate data sets describing equilibrium partition coefficients must be specified for the water column and the riverbed. First order degradation rates will be assigned for both the water column and sediment bed.

The evaluation of site-specific data for PCB concentrations, sediment grain size, and sediment organic carbon content raises the possibility of another mode of transport for the PCBs beyond the traditional PCB sorption process as a function of solids and/or organic carbon. This evaluation is ongoing, and when complete, the results may require the reassessment of the approach for modeling abiotic PCBs (see Figure 3-1).

4.2.3 AQUATOX

4.2.3.1 Overview

The AQUATOX model represents the combined environmental fate of conventional pollutants, such as nutrients, and contaminants in aquatic ecosystems. It has been used in modeling streams, ponds, lakes, and reservoirs. It incorporates several trophic levels, including attached and planktonic algae and submerged aquatic vegetation, zoobenthos and zooplankton, and

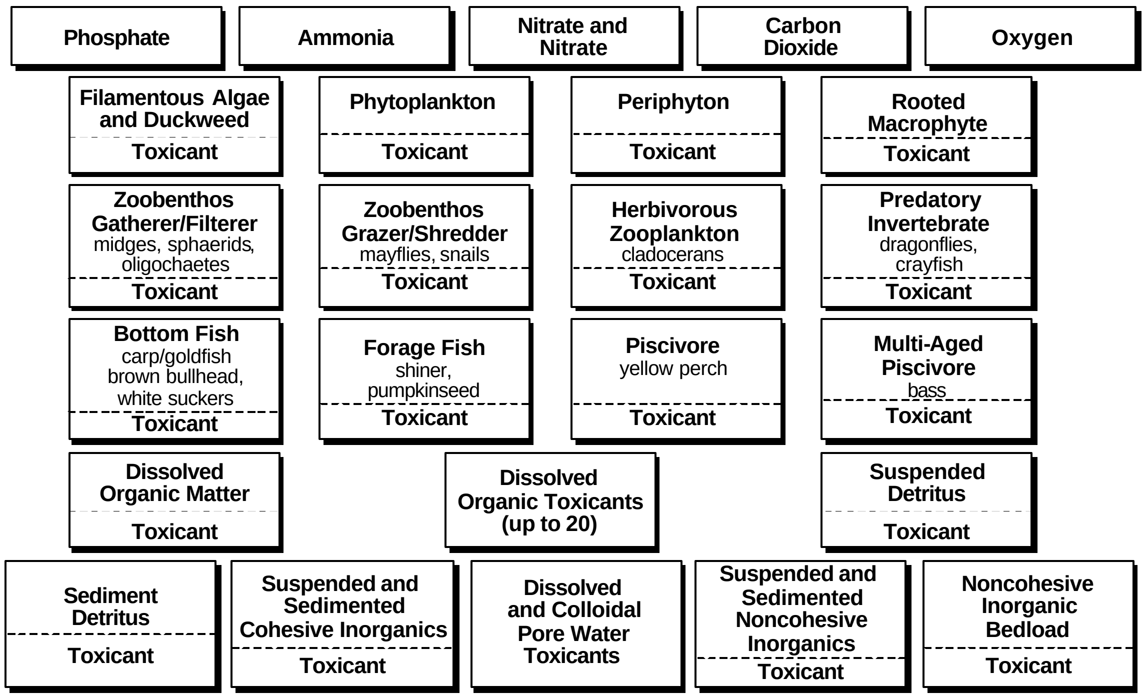


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Figure 4-6 Compartments (State Variables) in AQUATOX

forage, bottom-feeding, and game fish; it also represents associated organic contaminants (Figure 4-6). Relevant previous applications include validation with data on the fate and effects of pesticides in Minnesota and Israeli pond mesocosms (Park, 2000), verification with PCB data from East Fork Poplar Creek, Tennessee (Park, unpub.), and validations with PCB data from Lake Ontario and pesticide data from Coralville Reservoir, Iowa (EPA, 2000c).

AQUATOX represents the aquatic ecosystem (Figure 4-7) by simulating the changing concentrations (in g/m^3 or g/m^2) of organisms, nutrients, chemicals, and sediments in a unit volume of water or area of sediment. As such, it differs from population models, which represent the changes in numbers of individuals. As O'Neill et al. (1986) stated, ecosystem models and population models are complementary; one cannot take the place of the other. Population models excel at modeling individual species at risk and modeling fishing pressure and other age/size-specific aspects. However, recycling of nutrients, the fate of organic chemicals (Figure 4-8), and other interdependencies in the aquatic ecosystem are important aspects of a system such as the Housatonic River that AQUATOX represents, and that cannot be addressed by a population model.

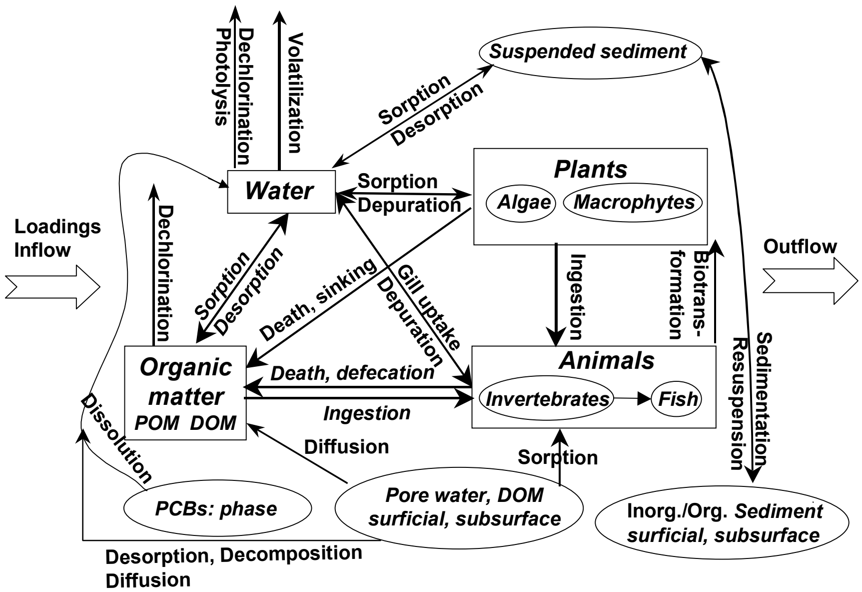

Figure 4-7 Fate and Bioaccumulation of PCBs

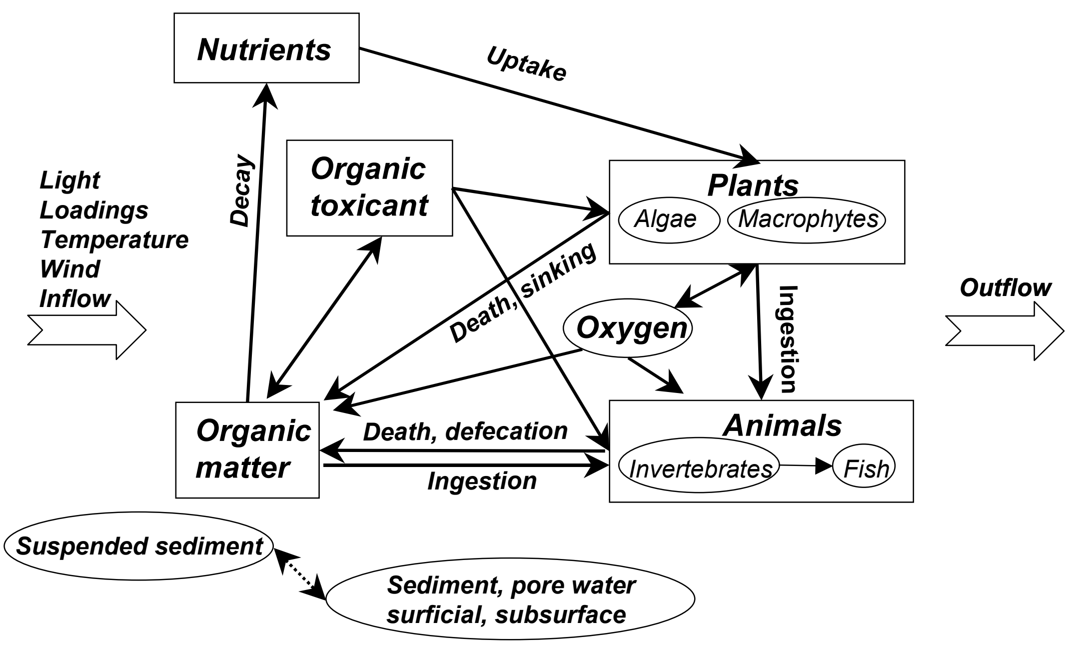

Figure 4-8 Processes Linking Ecosystem Components in AQUATOX

The model is written in object-oriented Pascal using the Delphi programming system for Windows™. An object is a unit of computer code that can be duplicated; its characteristics and methods also can be inherited by higher-level objects. This modularity is the basis for the flexibility of the model, including the ability to add and delete state variables interactively and to replicate the segment structure, providing the spatially distributed functionality required for this project.

The model has been optimized to address the specifics of PCB transfer in a riverine system. AQUATOX represents linked segments, including subreaches, backwater areas, and the epilimnion and hypolimnion in Woods Pond. Advection, diffusion, and migration link the segments. Two size classes can be represented for each fish species, and one species (largemouth bass) is represented by up to 15 age classes to better evaluate age-dependent bioaccumulation. As many as 20 chemicals or chemical groups, including PCB homologs or selected congeners, can be represented simultaneously. Up to 10 sediment layers and associated pore water can be simulated; the model is linked to the sediment transport module of the EFDC model. Animals can be parameterized to reflect their proportionate exposures to contaminants in pore waters and in the water column. Bioturbation is modeled as affecting the thickness of the active layer and biodiffusion.

The fate portion of the model is applicable specifically to organic contaminants such as PCBs. This portion includes kinetic partitioning among organisms, suspended and sedimented detritus, suspended and sedimented inorganic sediments, and water; volatilization; photolysis; biotransformation; and microbial degradation.

Temporal Resolution

Usually the reporting time step in AQUATOX is one day, but numerical instability is avoided by allowing the step size of the integration to vary to achieve a predetermined accuracy in the solution. This is a numerical approach, and the step size is not directly related to the temporal scale of the ecosystem simulation. AQUATOX uses a very efficient fourth- and fifth-order Runge-Kutta integration routine with adaptive step size to solve the differential equations (Press et al., 1986). The routine uses the fifth-order solution to determine the error associated with the fourth-order solution; it decreases the step size when rapid changes occur and increases the step size when there are slow changes, such as in winter. However, the step size is constrained to a maximum of 1 day so that daily contaminant loadings are always detected.

PCB Degradation and Loss

Biodegradation of contaminants such as PCBs is modeled as a maximum observed degradation rate (*Km*) modified for pH, temperature, and dissolved oxygen factors. Enhanced degradation under anaerobic conditions and elevated temperatures is explicitly modeled. Anaerobic *Km* values will be calculated for specific congeners, and hence proportionately for homologs that contain those congeners, using experimental data with microorganisms from Woods Pond obtained by Bedard and colleagues (Bedard and May, 1996; Van Dort et al., 1997; Wu et al. 1996, 1997a, 1997b). Bedard and May (1996) concluded that Aroclor 1260 accounted for at least 95% of the PCBs in Woods Pond—Aroclor 1254 accounting for no more than 5%—and that the congener distribution is the result of Processes N and P.

With 50 years of dechlorination, as Van Dort et al. (1997) assumed, and following the major routes of dechlorination postulated by Bedard and May (1996), *Km*s and half-lives can be computed for major components of Aroclor 1260. For example, based on the Bedard and May (1996) data, the computed half-life of the Cl_7 homolog group in Woods Pond is 129 years, with congeners 2345-2'4'5' being 168 years and 2345-2'3'4' being 92 years. It is beyond the sensitivity required for this application to model the N and P processes separately, so the rates will be based on the mean annual temperature, and seasonal temperature adjustments will be taken, recognizing that the overall optimal temperature of 30°C for PCB microbial dechlorination is higher than the maximum summer temperature of 22°C (Wu et al., 1996). Other studies will be used to estimate *Km* values for aerobic microbial degradation of lighter PCB homologs (for example, see Abramowicz, 1994).

The loss of an organic chemical through volatilization is modeled as a function of the Henry's Law constant for the compound, which is estimated using the HenryWin Ver. 3.02 program and compared with published values when available (Brunner et al., 1990; Dunnivant et al., 1992) and also corrected for ambient temperature. Volatilization also depends on the depth and flow rate of the river and wind speed, particularly for standing water such as Woods Pond. Volatilization can be a significant loss for the lighter PCB homologs. If appropriate, specific homologs and congeners be modeled separately.

PCB Sorption and Bioaccumulation

Sorption kinetics of PCBs involves dissolved and particulate organic matter and resulting bioavailability to biotic groups. Numerous studies have stressed the importance of distinguishing between truly dissolved PCB concentrations and dissolved and colloidal organic complexes because of differing bioavailability (for example, Landrum et al., 1985, 1987; Butcher et al., 1998). AQUATOX computes bioaccumulation factors with both truly dissolved and apparent dissolved chemicals to facilitate comparison with available data.

AQUATOX represents the kinetics of sorption and desorption, but the bioconcentration factors for biota (Figure 4-9) and steady-state partition coefficients for detritus are computed to indicate the maximum concentrations for direct uptake from a given dissolved level.

Computations are sped up by scaling and apportioning uptake relative to the maxima, thus avoiding numerical instabilities with competing rapid sorption processes. The partition coefficients, uptake rate constants, and depuration rate constants in AQUATOX will be calibrated using field observations on concentrations in sediments, water, and organisms, keeping in mind that a true steady-state is unlikely to occur in the river.

Exposure to PCBs is a function of diet, gill uptake, and direct sorption. The latter process is considered important for algae and macrophytes as discussed in the conceptual model. The sigmoidal curve for algal uptake in AQUATOX is being modified to account for steric effects in highly chlorinated homologs. AQUATOX allows the user to designate the proportions of overlying water and pore water that a given category of animal respires, and to account for exposure and nonlinear uptake through filtration activities. Prey preferences can be important for determining dietary exposures; the model weights available prey by specific predator preferences (using published values for the given fish species from rivers in the Northeast); this

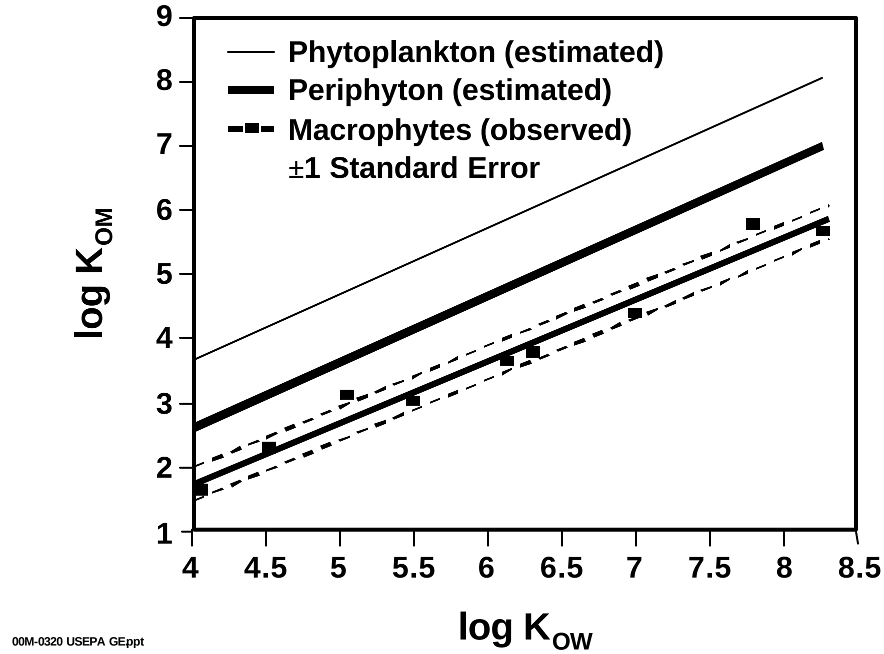

Figure 4-9 Steady-State Partition Coefficients in Plants

construct accounts for the reality of opportunistic and seasonally variable feeding. The gut absorption efficiency in AQUATOX is a function of the assimilation efficiency of the contaminated food, based on recently published observations (NIEHS, 1999) and similar to the approach taken in a bioaccumulation model for PCBs in the Upper Hudson River (QEA, 1999).

The model divides elimination into excretion and biotransformation. Loss of PCBs from algae by excretion and lysis is modeled explicitly. AQUATOX can be parameterized to represent degradation pathways in invertebrates and fish, including biotransformation from one congener to another. It is generally accepted that the *para* chlorines in the lower chlorinated congeners are readily hydroxylated and that biotransformation decreases with the degree of chlorination (Safe, 1980; Endicott and Cook, 1994). However, capacity for biotransformation varies by species; Gerstenberger et al. (1997) state that few fish exhibit P450 IIB1- and IIB2-type enzyme induction responsible for metabolizing lower chlorinated congeners (see also Bright et al., 1995). Given the ambiguity in the literature and the lack of definitive species-specific studies, site-specific data are being collected, and some degree of calibration will likely be necessary.

Modeling Endpoints

The model predicts concentrations of nutrients and dissolved and particulate detritus, biomass of various functional and taxonomic groups of organisms, concentrations of contaminants such as PCBs in the dissolved phase, and concentrations and bioconcentration factors associated with the detrital and biotic compartments. It also simulates control conditions, such as a no action alternative and a remediation alternative, in side-by-side runs. The output can be exported in database format suitable for post-processing.

4.2.3.2 AQUATOX Data Requirements

AQUATOX is designed to be run with varying quantities and qualities of data, depending on availability and purpose. In this modeling study, more than sufficient data are available for the calibration of most parameters. However, the historical Aroclor or total PCB tissue and sediment data from the 1980s are marginally adequate (and congener data are lacking) for validation, so more recent data for homologs and selected congeners will be used to validate the latter years of long-term simulations. The comparability of the analytical techniques used in generating the older PCB data with those used in more recent analyses is being evaluated to determine if older data can or need to be "adjusted" to account for any differences if they are used in this modeling study, analogous to the "tri+" approach that was necessary in the Hudson River modeling effort (Butcher et al., 1997).

As described in detail in Section 4.4.2, most of the estimated loadings and physical characteristics will come from HSPF and EFDC.

Physical Characteristics

For each segment, EFDC will provide to AQUATOX time-varying volume, surface area, mean depth, maximum depth, and cross-sectional area. Vertical diffusivity will be simulated and provided by EFDC for the epilimnion and hypolimnion of the deep hole of Woods Pond.

Ecosystem Loadings and Driving Variables

HSPF will provide time-varying loadings of NO_x, NH_4, PO_4, dissolved organic matter, and dissolved oxygen (mg/L) for each river segment to AQUATOX. EFDC will provide time-varying loadings of particulate organic matter, sand, silt, and clay (mg/L), inflow (m^3/d), and water temperature (EC) for each segment. Data obtained at the site will be used for time-varying solar radiation (Langleys/d), wind (m/s), and pH. The solar radiation will be corrected for seasonal riparian shading for each reach; wind will be important only for Woods Pond and will be corrected for height above water and shoreline sheltering.

Contaminant Loadings

HSPF will provide time-varying point-source and nonpoint-source loadings of PCBs (g/d or µg/L in inflow water) to AQUATOX.

Observations on Ecosystem Components

Data that have been or are being collected for the Supplemental Investigation for the AQUATOX river segments include biomass estimates for periphyton and macrophytes (g/m^2), phytoplankton (g/m^3), and invertebrates by functional or taxonomic group (g/m^2 or g/m^3), and fish by species (g/m^3), with measurement of length, weight, and for some species lipid content and age. Data also have been collected on concentrations of dissolved and particulate organic matter.

Observations on PCBs

Data have been or are being collected on concentrations of total PCBs and PCB congeners and homologs in the dissolved phase (µg/L), in sediment (µg/kg), associated with periphyton, phytoplankton, and macrophytes (µg/kg), in invertebrates (µg/kg), and in fish by species and size (µg/kg).

Chemical Parameters

Observed or estimated physicochemical and degradation parameter values are available for PCB homologs and selected congeners (see Table A-1 for examples). These include molecular weight, solubility, vapor pressure, Henry's Law constant, and octanol-water partition coefficients. Congener-specific microbial anaerobic degradation rates from Woods Pond will be used. Biotransformation rates are available for some congeners, and congener profiles in organisms are being generated specifically at the site. Henry's Law constants will be based on experimental values when available (e.g., Dunnivant and Elzerman, 1988; Dunnivant et al., 1988) and otherwise estimated using the Brunner procedure (Brunner et al., 1990).

Initial and Boundary Conditions

Calibration data from surface samples and cores (BBL, 1996; WESTON, 2000a) will be used to establish initial conditions for homologs and selected congeners in surficial and subsurface sediments. Body burdens in organisms will be set to 0, and the model will be run with average conditions and loadings for individual segments for several years to "spin up" simulated body burdens prior to the first observed fish data from the calibration period (Smith and Coles, 1997). Then time-varying concentrations in all compartments will be simulated for the period of 1995-2000 and compared to available data, both published and current.

Validation data from surface samples and cores (Stewart Laboratories, 1982) will be used to establish initial conditions for total PCBs in surficial and subsurface sediments. For purposes of the long-term validation, the proportions of homologs and selected congeners will be assumed to be those of the fresh Aroclors 1254 and 1260, with 1260 predominating (for example, see Bedard and May, 1996). Similar to the calibration, a steady-state spin-up period will be used to simulate bioaccumulation in fish prior to the first observed fish data in the validation period (Stewart Laboratories, 1982). Then homologs and selected congeners will be simulated from 1979 through 2000. Comparisons of predicted homologs and congeners will be made with more recent biotic and sediment data, and results will be converted to total PCBs and Aroclors to facilitate comparisons with older fish and sediment data.

The two upstream segments, the East and West Branches just above their confluence, will be used to define boundary conditions. They are short, low travel-time subreaches, so they will be simulated separately and linked to the downstream segments using the "cascade" advection scheme. Upstream loadings of total PCBs, provided by HSPF, will be split into homologs and key congeners according to observed ratios.

4.3 PHYSICAL DOMAINS OF COMPONENT MODELS

Each component model is applied to a particular physical portion of the Housatonic River watershed system, and at a spatial scale appropriate to the processes being simulated. In some cases, the physical domains overlap, to accommodate data and calibration issues. In other cases, the domains are coincident, but the spatial scales are different because of the differing physical, chemical, and biological processes of interest, the sensitivity of the calculations, and the computational efficiency of each model. In this section, the physical domains and spatial scales of each model are presented, starting with HSPF for the watershed hydrologic study area (HSA), followed by EFDC and AQUATOX for the PSA.

4.3.1 HSPF Housatonic Watershed Domain

As noted above, the physical domain of the HSPF model for this study is the entire watershed that drains to the gage at Great Barrington, MA, an area of approximately 282 square miles. This downstream boundary was selected because of the long-term flow record available (more than 80 years) for calibration. The watershed area at this point encompasses the entire PSA of the Housatonic River downstream from the GE facility at Pittsfield, the area in which historical data suggest that the majority of PCB-contaminated sediment and floodplain soil is located.

Whenever HSPF, or any watershed model, is applied to an area of this size, the entire study area must undergo a process referred to as "segmentation." The purpose of watershed segmentation is to divide the study area into individual land and channel segments, or pieces, that are assumed to demonstrate relatively homogenous hydrologic/hydraulic and water quality behavior. This segmentation then provides the basis for assigning similar or identical parameter values or functions to where they can be applied logically to all portions of a land area or channel length contained within a segment. Since HSPF and most watershed models differentiate between land

and channel portions of a watershed, and each is modeled separately, each undergoes a segmentation process to produce separate land and channel segments that are linked together to represent the entire watershed area. The initial watershed and channel segmentation of the Housatonic River watershed are discussed separately below. The initial segmentation is shown in Figure 4-2.

4.3.1.1 Watershed Segmentation

Watershed segmentation is based on individual characteristics of the watershed, including topography, drainage patterns, land use distribution, meteorologic variability, and soil conditions. The process is essentially an iterative procedure of overlaying these data layers and identifying portions of the watershed with similar groupings of these characteristics. Over the past decade, the advent of geographic information systems (GIS) and associated software tools, combined with advances in computing power, have produced automated capabilities that can efficiently perform the data-overlay process.

For the Housatonic River watershed, the topographic and drainage pattern analysis for subbasin delineation was performed using the tool AVSWAT (Di Luzio et al., 1998), which produces map layers of subbasins and river segments using a digital elevation model (DEM) grid as input. AVSWAT automatically defines subbasins based upon a user-specified threshold number of grid cells, but it also allows the user to specify locations as subbasin outlets. For this application the DEM from the BASINS system (Lahlou et al., 1998), with a resolution of 100 meters, was used to define 39 separate subbasins within the Housatonic River watershed down to Great Barrington, MA. These subbasins range in size from 0.4 to 23.8 mi^2, and include stream reaches that range in length from 0.6 miles to 8.8 miles. The land and channel segmentation will require further refinement to produce a reasonable representation of the watershed consistent with the EFDC grid and the AQUATOX segments. The guidelines followed and issues encountered in producing the segmentation shown in Figure 4-4 are outlined below:

1. Two of the model segments were defined with outlets at the USGS gaging stations at Coltsville and Great Barrington to facilitate hydrologic calibration to the available flow data at these sites.

2. The threshold level of aggregation of grid cells with AVSWAT was adjusted to define channel locations that extended throughout most of each subbasin so that the drainage pattern within each segment would be adequately represented.

3. The segment division that corresponds to the 10-year floodplain between Dalton and Woods Pond was designed to correspond to the river segments defined in the Supplemental Investigation Work Plan (WESTON, 2000a); thus, WESTON river Reach 1 corresponds to HSPF reach No. 1000, WESTON Reach 2 corresponds to HSPF reach No. 2000, etc. Also, model segments that drain to these reaches were numbered consistently so that segments with numbers in the 100s contribute to WESTON Reach 1, segments labeled in the 200s contribute to WESTON Reach 2, etc.

4. Although the SI Work Plan defined a single reach from the confluence of the East Branch and West Branch to Woods Pond, a finer segmentation was imposed in this region to provide better spatial definition for this reach for both the hydrology calibration and the linkage with AQUATOX (discussed below).

5. In areas with very flat slopes and/or incised channels, the watershed-scale DEM resolution was not sufficient to accurately define the channel location, such as between the confluence of the East Branch and West Branch and Woods Pond, and downstream of Coltsville. In these cases, the USGS maps and the EPA RF3 stream coverages were used to properly define the channel locations.

AVSWAT also generates tables of attributes with each map layer. The subbasins were overlayed with the land use data to determine the area of each land use contributing to each river segment. This analysis was performed using the land use coverage from BASINS along with the ArcView GeoProcessing Tool. The BASINS land use data layer (circa 1980-84) includes 17 different land use categories, which were combined, using the AVSWAT tool, into seven groups for simulation.

The seven AVSWAT land use groupings provide the basis for selecting categories for simulation within each subbasin with HSPF. Since the focus of the HSPF component in this study is on sediment, PCB, and nutrient loadings, we will simulate only four of the seven land use categories: urban, forest, agriculture, and wetlands. Appendix E includes tables with the land use areas for each of the seven AVSWAT categories for each subbasin. The overall land use distribution for the entire watershed area at Great Barrington is as follows:

Urban	15.0 %
Agriculture	10.8 %
Forest, Deciduous	39.1 %
Forest, Evergreen	28.2 %

Forest, Mixed	1.1 %
Lakes/Reservoirs	1.8 %
Wetlands	4.0 %

Appendix E also includes subbasin areas, elevations, and slopes all derived from the DEM data using the AVSWAT tool.

Although the land use coverage available for the site was generated in the early 1980s, the predominant rural/agricultural nature of the entire watershed has not significantly changed since that time. However, further evaluation of the urbanization of the watershed is being performed and any changes identified in specific model segments will be incorporated into the land use coverage.

4.3.1.2 Channel Segmentation

Segmentation of the channel was also performed with the AVSWAT tool because it uses DEM data to determine drainage divides and stream locations for the mainstem and all tributaries. In this approach, a single HSPF stream or channel reach within each subbasin was included as shown in Figure 4-2. Since detailed hydrodynamics and sediment transport will be performed by EFDC, and detailed PCB simulations will be performed by AQUATOX, the stream simulation in HSPF is performed primarily to allow calibration at the primary sampling locations along the river. Appendix E shows stream channel attribute data, including the subbasin in which the channel resides, the downstream subbasin, reach length, elevation drop across its length, and slope. This information summarizes the initial physical characterization of the channel system; however, the DEM resolution may be too coarse to generate accurate information; the generated channel data will be evaluated against the detailed cross-section data collected for the mainstem to define the EFDC grid (discussed below) and revised if necessary.

4.3.2 EFDC Housatonic River and Floodplain Domain

4.3.2.1 Introduction

As discussed above, the EFDC model will be used to simulate hydrodynamics, solids transport, and abiotic PCB fate and transport in the Housatonic River, and will simulate overbank transport of water and solids into the associated floodplain. Using available shoreline, channel cross-section, bathymetry, and floodplain elevation data, the physical domain of the Housatonic River will be spatially discretized into a computational scheme as a (a) boundary fitted, orthogonal, curvilinear, (b) cartesian, or (c) nested or hybrid grid consisting of a fine-scale grid representing the main channel and a coarse-scale grid representing the floodplain region.

Specification of an appropriate grid scheme is critical to properly representing the external and internal forces occurring and their influence on the transport of both sediment and PCBs in a river with characteristics such as those of the Housatonic. A grid representing the physical domain of the study area provides the computational framework by which resulting forces are translated throughout the system in terms of both magnitude and direction. The physical complexity of this system presents challenges, where neither a cartesian nor a curvilinear-orthogonal grid is easily fitted to the shoreline boundary.

The complexity of this system requires a strategy to determine the grid scheme that will result in a scientifically credible, yet computationally feasible model. The strategy must provide a framework for evaluating the compromise between depicting the physical realities of the river and floodplain system and computational feasibility. This section presents the proposed strategy and rationale for determining an optimal grid configuration.

A key consideration in defining an optimal grid configuration is the need to aggregate outputs from a fine grid used for the hydrodynamic and sediment transport to the coarse grid used by the PCB fate and bioaccumulation model. Consequently, the strategy must include a means of determining whether artificial biases are introduced into the modeling analysis as a result of using different grid configurations and/or as a result of the process of spatial and temporal aggregation between different models.

There are two distinct physical domains that need to be modeled in this system. The first physical domain is the main river channel and associated 10-year floodplain between the USGS station at Coltsville to the upstream influence of the backwaters of the Woods Pond Dam. The domain of this model will be referred to as the Riverine/Flood Plain (R/FP) Model. The second physical domain is the Woods Pond impoundment and its backwaters, which will be referred to as the Woods Pond (WP) Model. Because of their differing characteristics and needs, the two physical domains will be represented in EFDC using two separate coupled grid schemes. The downstream boundary of the R/FP Model will be set at a location defined by the farthest upstream influence of the backwater resulting from the Woods Pond Dam. Downstream boundary time-series results of the R/FP Model (stage height, flow, solids loading, abiotic PCB loading) will be coupled as the upstream boundary for the WP Model. Each model domain will thus have its own grid scheme to represent the major differences in the two physical domains. An additional benefit realized by this approach is a better coupling with the AQUATOX segmentation.

Unlike the difficulties that are discussed below for the numerical grid representation of the main river channel of the R/FP Model, spatial discretization of the Woods Pond and backwater region represents a situation more typical of the traditional applications of a curvilinear or cartesian grid for open-water systems such as lakes, estuaries, or coastal waters. Fitting either a curvilinear or cartesian grid scheme to the WP Model does not require the same level of testing as described below for the R/FP model. For the WP Model, a 3-D cartesian grid using variable horizontal cell sizes (e.g., 5 to 20 m) and three to seven vertical layers as a “sigma” coordinate system is proposed for Woods Pond and its backwater areas. The vertical resolution envisioned in Woods Pond is intended to address such issues as thermal stratification that occurs in the deeper regions of Woods Pond during summer.

The remainder of this section presents a discussion of the strategy proposed to address computational issues associated with the spatial discretization of the complex physical domain of the main river channel and floodplain for the R/FP Model necessary to realistically depict the processes within the Housatonic River PSA.

4.3.2.2 Technical Strategy for Developing an Optimal Grid Scheme for the R/FP Model

The strategy that will be used to determine the optimal grid configuration achieves a balance beween the representativeness and computational feasibility involves of a representative section of the river referred to as the “test reach.” Figure 4-10 shows the test reach and its location just upstream of New Lenox Road. For the test reach, a series of coarse to highly refined cartesian grids and a range of nested grids will be evaluated.

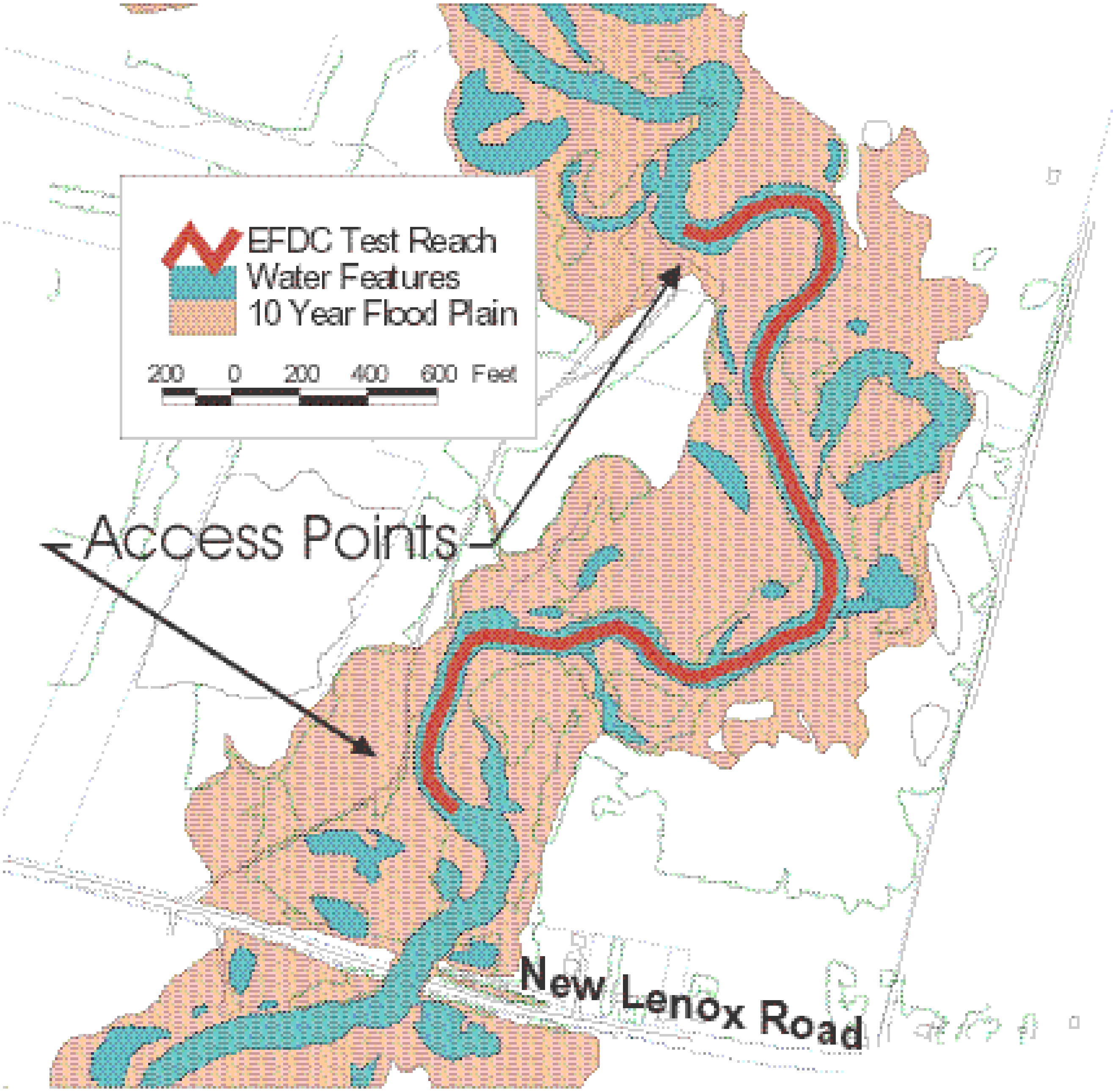

Figure 4-10 EFDC Test Reach Location

Testing will be performed to find the most appropriate grid scheme and spatial scale for the R/FP Model to address the concerns discussed above.

Results from the evaluation of alternative methods will be compared to detailed site-specific field measurements of flow, velocity, stage height, and TSS (total, cohesive and noncohesive size fractions). Through an iterative process, the resolution of each test case will be progressively coarsened through subsequent simulations to evaluate the effects associated with the loss of information accompanying the loss of spatial resolution. Once significant errors or differences occur between simulations, the prior cell size will be identified as the "appropriate" discretization for that scheme. The ease of application and computational requirements for each of type of grid scheme will be evaluated and a final grid scheme and discretization will be selected for the entire study area.

Technical issues that will be evaluated using the test cases include examining the potential resolution of (1) "staircase" transport in reaches where the sinuous channel is not oriented with the N-S and E-W alignment of the faces of the cartesian cells; (2) lateral transport and resuspension and deposition of solids in reaches characterized by highly sinuous meanders; and (3) interaction of flow between the river channel and the floodplain during bankfull flows in the various test case scenarios.

***Staircase Transport*—**The presence of meanders is characteristic of natural rivers and represents the most stable channel configuration. The PSA of the Housatonic River exhibits this pattern of complex sinuosity. One option identified above is superimposing a cartesian grid scheme on the system and attempting to preserve the natural sinuosity of system by identifying "active" cells that are reasonably aligned with the main channel. There are difficulties in precisely mapping a cartesian grid to a naturally meandering system. As shown in Figure 4-11, this usually results in "staircase" transport where flows are periodically routed through alternating N-S to E-W to N-S cells. The extent to which abrupt changes in the direction of flows introduce errors into the momentum terms of the hydrodynamic solution needs to be carefully evaluated in the test cases.

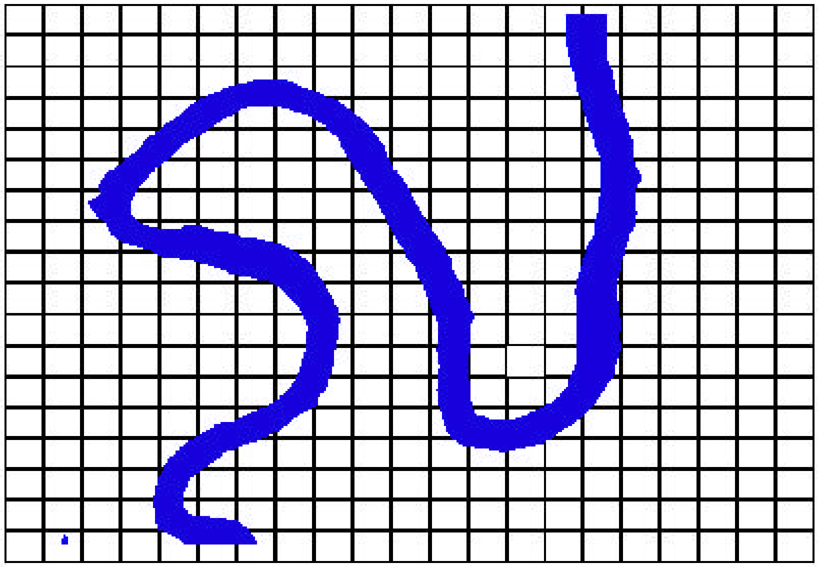

Figure 4-11 Sample Cartesian Grid

As an alternative, a boundary-following curvilinear grid may be developed to provide the most accurate simulation of fine-scale hydrodynamic processes and act as a benchmark to compare results from the cartesian grid test cases.

Lateral Transport in Meanders**—**Physical transport processes within meandering rivers are inherently complex, with erosion occurring as expected along the exterior or outer bank and deposition occurring on the interior or inner bank. In any channel meander, the velocities in the downstream direction of flow are dependent on the path length, with slower velocities occurring at the inner bank and faster velocities occurring at the outer bank. The differences in lateral velocity distribution across a channel directly influence the sediment transport capacity within the channel. Therefore, the significance of this lateral gradient must be evaluated in establishing an optimal grid scheme. Using a single lateral cell in any grid to represent a portion of the main channel is equivalent to treating sediment transport as being uniform across the channel, in effect eliminating this process. If the lateral variation in solids transport is not considered, then the model could potentially generate a systematic error in the solids balance (and hence PCB mass balance). An additional concern arises in those instances where net solids deposition or erosion is occurring, as would be expected on the inner and outer sides of the meander, respectively. The model would treat the entire cell as being in either net depositional or erosional, which may or may not be a realistic representation of the overall solids and PCB mass balances. The implementation of the proposed strategy using different scales of spatial resolution and exploring different boundary-fitted and cartesian grid schemes will test the significance of representing portions of the main channel as a single cell in comparison to representing the river channel with multiple lateral grid cells.

Interaction of Flow Between Channel and Floodplain**—**Because the floodplain within the PSA is known to contain elevated levels of PCBs (up to 800 ppm detected), the interaction of out-of-bank flow between the river channel and the floodplain must be represented in the model to achieve mass balance and to accurately represent the distribution of solids and PCBs between the channel and floodplain, particularly under high-flow conditions. For this study, the extent of the 10-year floodplain will be represented in the physical domain of the model as a 2-D network of "wetting and drying" grid cells.

The spatial resolution necessary to represent out-of-bank flows onto the floodplain must be evaluated within the scale of the 10-year floodplain to preserve the observed conditions, yet ease the computational load. For example, a uniform 20-m x 20-m cartesian grid superimposed on the 10-year floodplain would require on the order of approximately 13,000+ "wetting and drying" cells within the PSA. Such a scheme raises concerns about computational feasibility. On the other hand, there is a concern that if too coarse a cell size is used to represent the main channel, then a significant loss of physical process information could result. This issue has been addressed successfully in the Florida Everglades using a nested-grid approach (Hamrick, 1994b).

A nested-grid approach in which the floodplain is represented by a coarse cartesian grid scale and the river channel defined by a "nested" curvilinear grid as a subgrid scale model will also be evaluated for the Housatonic River. In the nested grid, the subgrid interacts with the larger scale "host" cells via exchange flow at the boundaries of the coarse floodplain grid cells (Hamrick and Moustafa, 1999a, 1999b; Moustafa and Hamrick, 2000). If it can be demonstrated that a dual grid strategy can provide a reasonable simulation for coupling channel flow with the floodplain under flood conditions, by comparison to the results generated from a uniform cartesian grid resolution model as well as observed data, then significant computational efficiencies can be realized in applying a nested-grid scheme for the physical domain of the Housatonic River floodplain for the EFDC model.

4.3.3 AQUATOX Domain

The AQUATOX model will be used to simulate the fate and bioaccumulation of PCBs and, if necessary, other toxic organic contaminants in the PSA. This aquatic ecosystem model will be applied to the main channel, Woods Pond, and the backwater areas of Woods Pond. Overbank conditions during flood stage will not be simulated because floodplain processes are not included in AQUATOX. The following segments, including subreaches of the Housatonic River and subdivisions of Woods Pond, will be simulated in AQUATOX with linkages to HSPF and EFDC described in detail in Subsection 4.4:

Reach 4a: Pomeroy Avenue Bridge to Confluence. This segment provides the upstream East Branch boundary conditions for simulating both the ecosystem components and the organic contaminants. This segment begins approximately 2 miles downstream from the GE facility and provides the external loadings from the East Branch for the simulations. Segment 4a is also downstream of the channelized reach and represents the beginning of the natural river channel.

Reach 4b: West Branch Housatonic River. This segment forms the other upstream boundary condition, on the West Branch. There is appreciable flow and adequate aquatic habitat in the West Branch or impoundments upstream. In addition, during the course of the Supplemental Investigation, PCBs were detected in the West Branch; further investigation is ongoing.

Reach 5a: Confluence of West and East Branches to Wastewater Treatment Plant. Shallow, meandering, free-flowing, and with little human alteration, this subreach represents the first depositional area for finer grained sediments (up to 10% silt and clay) and PCBs. Snags (larger woody debris) and bars are common features.

Reach 5b: Wastewater Treatment Plant Discharge to Roaring Brook. This subreach receives effluent from the Pittsfield Wastewater Treatment Plant. It is a dynamic, graded stream with numerous active meanders and backwater areas. Macrophytes become more abundant in the shallow channel, and abundant algae and zoobenthos reflect the enriched habitat.

Reach 5c: Roaring Brook to Woods Pond. In contrast to Reach 5b, this subreach is characterized by a slower-moving river that occupies a more stable channel due to the influence of the Woods Pond Dam. The banks of the river are more heavily wooded in stretches, and the channel has many deep runs and pools (7 ft or more in depth). Organic content of the sediments is greater than upstream, and the fauna is diverse.

Reach 6a: Deep Channel Immediately Upstream from Woods Pond. The channel deepens as it reaches the inundated floodplain just upstream of Woods Pond proper. The low floodplain broadens, with a marked increase in macrophytes and algae during the growing season.

Reach 6b: Backwater Areas Immediately Upstream from Woods Pond. Extensive, very shallow areas of inundated floodplain occur just upstream of Woods Pond. These are prime macrophyte and zoobenthos habitat, and also provide habitat for assemblage of biota that prefer shallow, still water. Although somewhat isolated from the flow of the river, these backwaters do receive sediments and associated contaminants during high-flow conditions, as demonstrated by the PCB concentrations observed in sediment. The backwater areas will be modeled as a single composite segment accounting for the total surface area and volume.

Reach 6c: Deep Hole in Woods Pond. The eastern portion of Woods Pond was the pre-impoundment meander of the river, currently inundated, and has a maximum depth of 16 ft in thickness. It is also an area of sediment deposition of up to 16 ft. It is stratified during the growing season and will be modeled as two segments—epilimnion and hypolimnion. It supports a typical eutrophic pelagic ecosystem.

Reach 6d: Shallow Portion of Woods Pond. The western segment of Woods Pond, although in line with the upstream river channel, is a very shallow (1 to 2 ft deep), inundated pre-impoundment floodplain. It is similar to Reach 6c in that it supports a typical eutrophic pelagic system as demonstrated by the predominant cover of dense macrophytes and filamentous algae. This shallow area has between 3 to 6 ft of sediment accumulation as measured by the refusal depth of hammer-driven probes.

4.4 MODEL LINKAGE

4.4.1 Introduction

The integrated modeling framework described in Section 4.1 was developed because no single model is capable of representing all the relevant physical, biogeochemical, and biological processes that operate over a wide range of time and space scales to influence the distribution of PCBs in the water column, sediments, and biota of the Housatonic River. The design of a methodology for linkage of inputs and outputs among the models requires consideration of both spatial and temporal issues, since all three models simulate different processes at different time and space scales. The physical domains of each model and the resulting transfer of information (i.e., model results) must be closely integrated to allow for the efficient operation and effective representation of the Housatonic River watershed system.

4.4.1.1 Overview of Model Linkage

Figure 4-12 illustrates an overview of the linkage of the outputs from the watershed model (HSPF) as water inflows and constituent loads from nonpoint sources (drainage basin runoff) and point sources (tributaries and wastewater dischargers), to the hydrodynamic and sediment transport model (EFDC), and the PCB fate and bioaccumulation model (AQUATOX). Figure 4-12 also shows an overview of the linkage of the output from EFDC as inputs of water inflows, reach geometry, and solids loads to AQUATOX. HSPF will provide AQUATOX with water temperature and point and nonpoint source loads for inorganic phosphorus (as P), nitrate+nitrite (as N), ammonia (as N), dissolved oxygen, water temperature, BOD, organic matter, and PCBs. HSPF will provide EFDC with point and nonpoint source inpus for steamflow, water temperature, and loads for total suspended solids and total PCBs. EFDC will provide AQUATOX with streamflow, reach geometry (volume, surface area, cross-sectional area), and loads of inorganic solids.

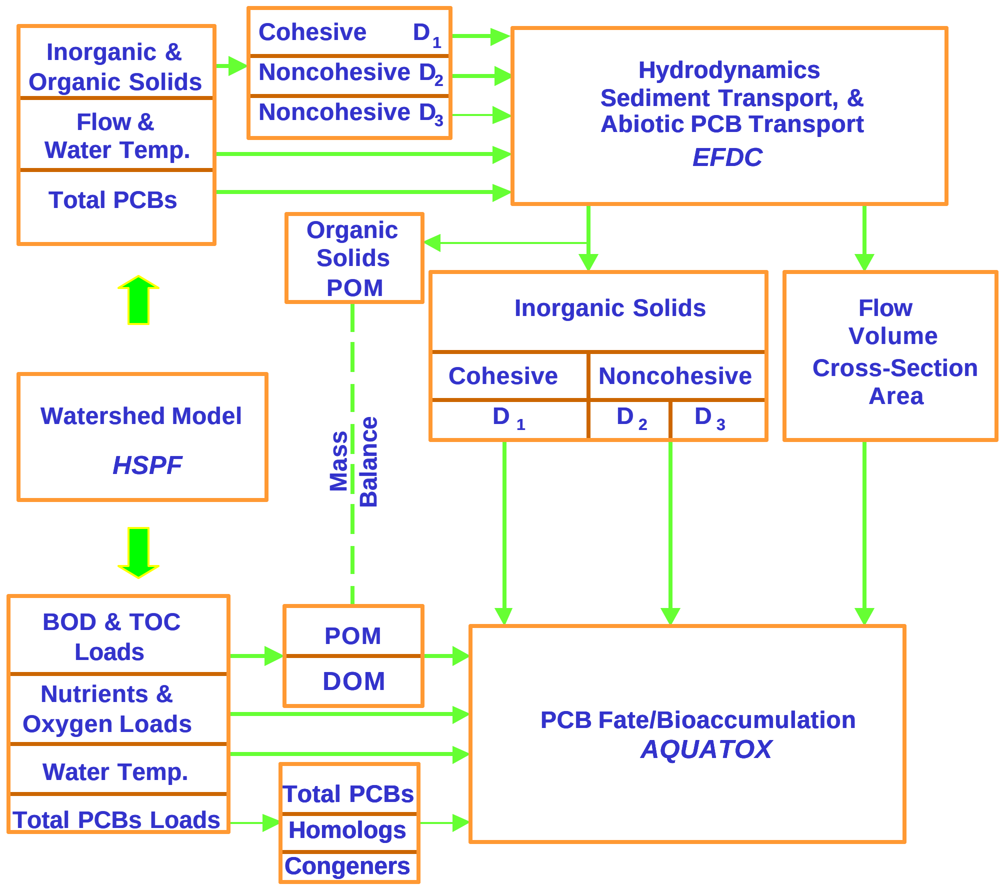

Figure 4-12 Overview of Model Linkage and Data Transfers within the Modeling Framework for HSPF, EFDC, and AQUATOX

Using streamflow, water temperature, solids, and PCB loading data provided by HSPF, EFDC will simulate water temperature, velocity, stage height, and streamflow in the hydrodynamic model; cohesive and noncohesive size classes of solids in the sediment transport model; and PCBs in the abiotic PCB transport and fate model. Using streamflow, reach geometry, and inorganic solids loading data provided by EFDC, AQUATOX will account for inorganic solids in the water column and simulate evolution of the sediment bed based on erosion and deposition fluxes of solids provided by EFDC. Using water temperature and the loading data provided directly by HSPF, AQUATOX will simulate organic matter, dissolved oxygen, inorganic nutrients, and trophic levels of biota that include algae, macrophytes, benthic invertebrates, and fish. AQUATOX will simulate homologs and selected congeners of PCBs in the water column and sediment bed and bioaccumulation in the biota.

4.4.1.2 Spatial Scales

As shown in Figure 4-12, the framework for the three models reflects a "nested" model approach with each model defined by a physical domain and relevant spatial and temporal scales. Within the physical domain of AQUATOX, the river is represented by a series of coarse-scale, single-layer, cascading reaches for the mainstem of the river, and a coarse-scale network of interconnected, two-layer reaches for the backwater areas of the river and Woods Pond. Within the physical domain of HSPF, the spatial scale of the mainstem of the Housatonic River is designed to overlay identically with the spatial scale of the reaches specified for AQUATOX. The procedure for linkage of pollutant loads from HSPF to AQUATOX is straightforward because all the nonpoint source loads and point source loads generated within an HSPF reach of the Housatonic River will be input at the upstream boundary of the corresponding AQUATOX reach.

The hydrodynamic and sediment transport model (EFDC) represents the finest resolution of spatial scale of the model framework. As discussed above, it is represented by two coupled models: (1) river/floodplain (R/FP) and (2) Woods Pond and backwaters (WP).

The procedure for the linkage of streamflow, reach geometry, and solids loads from EFDC to AQUATOX is less straightforward since the mass fluxes (i.e., [flow] x [concentration]) of water and solids simulated within each EFDC grid cell of the river channel and Woods Pond must be summed horizontally and vertically over the boundaries of each AQUATOX R/FP reach and WP segment. The horizontal flux of water and solids is summed for each grid cell across the upstream boundary to define the upstream input to each AQUATOX R/FP reach and WP segment. The export (or import) of fluxes of water volume, solids, and PCBs between the river channel and floodplain will be tracked by summing the fluxes over each grid cell along the floodplain/channel boundary.

Because the domain of AQUATOX does not include the floodplain, fluxes of water volume and solids to/from the floodplain must be computed and tracked to maintain the mass balance of water and solids provided from EFDC to the AQUATOX R/FP reaches and WP segments. In the WP model, the vertical fluxes of water volume and solids deposition and solids resuspension are summed over the array of grid cells corresponding to each AQUATOX segment to define the total vertical flux for input to AQUATOX.

4.4.1.3 Time Scales

Using high-frequency meteorology and upstream streamflow as input data, HSPF generates streamflow, water temperature, and constituent loads on a time scale of hours. Hourly time series of streamflow, water temperature, and solids loading data provided by HSPF as input to EFDC are linearly interpolated in EFDC to match the very high frequency time step (~minutes) needed for the hydrodynamic model. The output results of EFDC are written to external files for post-processing at a high-frequency interval (e.g., 1 to 2 hrs) designed to capture the hydrodynamic and sediment transport processes associated with the runoff hydrograph of storm events. In contrast to both HSPF and EFDC, AQUATOX is designed to represent the behavior of physical, chemical, and biological processes operating on a low-frequency time scale. With a daily time scale used to define inputs of streamflow and pollutant loads and resulting ecological processes, AQUATOX can resolve changes that are detectable over a monthly to seasonal time scale. To link output data sets from HSPF and EFDC as input time series to AQUATOX, the high-frequency results from HSPF and EFDC are numerically integrated over a 24-hour period to generate daily time series for input to AQUATOX.

4.4.1.4 Relationship of Modeling Framework Design and Modeling Study QAPP

The following section (4.4.2) presents a detailed description of the methodology used to construct the data linkages for the model framework, HSPF, EFDC, and AQUATOX. The Modeling Study QAPP (Beach et al., 2000) presents a detailed description of QA/QC procedures proposed to ensure that the linkages between HSPF, EFDC, and AQUATOX are performed correctly. The driving principle in designing QA/QC procedures for testing the model linkages is the requirement to maintain a mass balance of water, solids, nutrients, and PCB loads provided to AQUATOX by HSPF and EFDC.

4.4.2 Linkage Methodologies

The details of the methodologies adopted for linkage of the three models are described in this section. The discussion accompanying the variables listed below is intended to provide the necessary information for evaluating the adequacy of the methodology proposed for linking HSPF and EFDC output as input to AQUATOX, and is intended to address the following issues:

- What point and nonpoint source loads are generated by HSPF?
- How are HSPF loads linked to AQUATOX?
- How are HSPF loads linked to EFDC?
- How are EFDC fluxes linked to AQUATOX?
- What I/O transformations are used?
- What field data are used to support I/O transformations?

The discussion is organized by related groups of state variables as follows:

- Streamflow, water temperature, and reach geometry
- Inorganic nutrients and dissolved oxygen
- Solids, BOD, and organic matter
- PCBs

4.4.2.1 Streamflow, Water Temperature, and Reach Geometry

Figure 4-13 illustrates the linkage of nonpoint and point source inputs of flow generated by HSPF with EFDC and AQUATOX. This section describes the methodology that will be used to link streamflow, water temperature, and reach geometry data provided by HSPF and EFDC and the transformation of these data necessary to maintain a correct water balance and heat balance, and reach volume, depth, cross-sectional area, and surface area for input to AQUATOX.

HSPF

Driven by time-series input of precipitation and upstream boundary inflows, the HSPF watershed model generates high-frequency streamflow based on hydrologic processes describing surface runoff and subsurface inflow as nonpoint source inputs and flow routing in the tributaries as point source inflows. A one-dimensional transport model is used in HSPF for in-stream routing of flow in the mainstem of the Housatonic River and its tributary reaches. Based on climatology

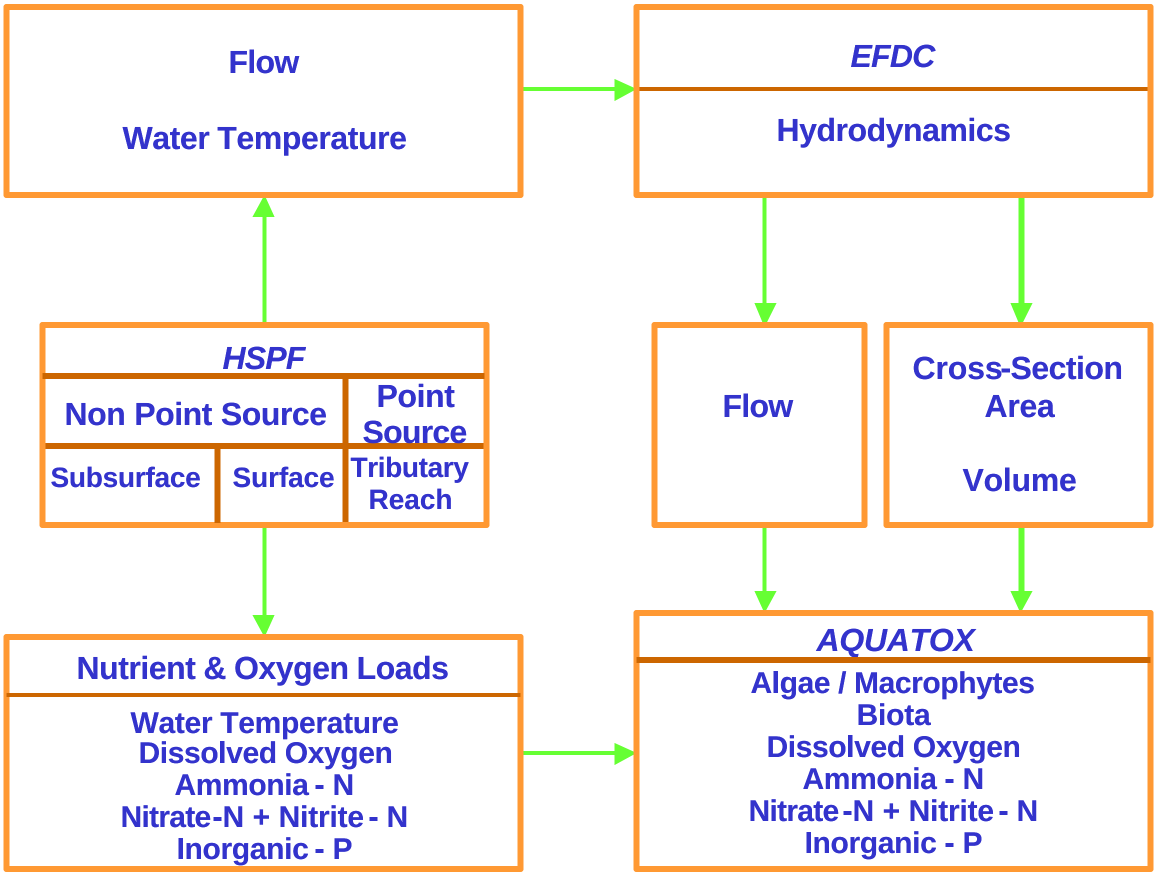

Figure 4-13 Model Linkage Within the Modeling Framework for Flow, Reach Geometry, Water Temperature, Inorganic Nutrients, and Dissolved Oxygen

and meteorologic time series data, a one-dimensional heat balance model is used in HSPF to simulate water temperature in the mainstem and tributary reaches of the watershed model.

HSPF-EFDC

Surface and subsurface inflows generated by HSPF as nonpoint runoff are distributed to each EFDC grid cell in proportion to the length of the grid cell and the length of the HSPF mainstem reach. Point source inputs of flow and water temperature contributed by tributary inflows and wastewater discharges are input to specific EFDC grid cells corresponding to the spatial location of the tributary or wastewater discharge. Hourly time series of streamflow and water temperature data provided by HSPF for input to EFDC are linearly interpolated in EFDC to match the high-frequency time step (~minutes) needed for the hydrodynamic model. For both nonpoint and point sources, flow and water temperature are specified for input to EFDC grid cells as time series data sets to define boundary inflows as follows:

Boundary inflow of water…………………………………………………..(m^3 sec^{-1})
Water temperature……………………………………………………………(^oC)

EFDC-AQUATOX

Driven by the boundary inflows of water provided by the watershed model, the hydrodynamic model simulates water temperature, stage height, velocity, and streamflow in the coupled R/FP and WP models. Streamflow is summed over the EFDC grid cells across the upstream boundary and the channel/floodplain boundary of each matching AQUATOX R/FP reach and each WP segment. In the WP model, mean horizontal and vertical dispersion coefficients are computed for the set of EFDC grid cells to define: (a) mixing across horizontal interfaces; and (b) mixing between the epilimnion and hypolimnion of each two-layer AQUATOX segment. Time series of upstream streamflow, floodplain/channel flow (to/from), and vertical and horizontal mixing coefficients are numerically integrated over a 24-hour period for input to AQUATOX as daily time series.

Grid cell volumes and surface areas are spatially summed over the horizontal array of EFDC grid cells that correspond to each AQUATOX reach in the R/FP model and each AQUATOX segment in the WP model. Time series of spatially summed cell volumes and surface areas are numerically integrated over a 24-hour period for input to AQUATOX as daily time series to define reach geometry. Using the low-frequency daily time series of volume and surface area and assuming the reach/segment computational volume is defined as a rectangular box, the mean depth and mean cross-sectional area are computed from the following ratios:

Reach Depth = Reach Volume/Reach Surface Area……………………………….Eq. (4-1)
Reach Cross-Section Area = Reach Volume/Reach Length……………………….Eq. (4-2)

EFDC provides AQUATOX with the following reach geometry and transport parameters as daily time series:

Volume……………………………………………………………………………..(m^3)
Cross-sectional area at upstream-downstream interfaces………………………………..(m^2)

Surface area (horizontal)……………………………………………………………(m^2)
Horizontal flow at upstream boundary……………………………………………..(m^3 day^{-1})
Horizontal flow to/from channel/floodplain……………………………………..(m^3 day^{-1})
Horizontal dispersion rate for WP interfaces………………………………………(m^2 day^{-1})
Vertical dispersion rate for WP eplimnion-hypolimnion…………………………..(m^2 day^{-1})

4.4.2.2 Inorganic Nutrients and Dissolved Oxygen

Figure 4-13 also illustrates the linkage of nonpoint and point source loads of nutrients and dissolved oxygen generated by HSPF as input to AQUATOX. This section describes the methodology that will be used to link nutrients and dissolved oxygen provided by HSPF to AQUATOX. There is no linkage between HSPF and EFDC for inorganic nutrients and dissolved oxygen.

HSPF

HSPF generates inorganic nutrients and dissolved oxygen with the simulated loads calibrated to observed water quality data collected in the tributaries and at mainstem stations of the Housatonic River. Inorganic nutrient loads generated by HSPF account for nitrogen as ammonia-N, nitrite-N plus nitrate-N, and phosphorus as orthophosphate-P. The organic forms of nitrogen and phosphorus are represented as the nutrient equivalents (nitrogen: dry weight; phosphorus: dry weight) of particulate organic matter (as dry weight). HSPF generates nonpoint source loads of nutrients and dissolved oxygen delivered to the edge of a stream as subsurface inputs and surface runoff over the incremental drainage area between tributary reaches. Surface runoff loads of dissolved oxygen are based on 100% saturation. Subsurface inputs of oxygen are based on mean monthly concentrations observed in groundwater.

A one-dimensional water quality model is used in HSPF for instream advective routing with kinetic sources and sinks of nutrients and oxygen simulated in the mainstem and tributary reaches. Kinetic processes for dissolved oxygen include atmospheric reaeration, decomposition of BOD and total organic carbon, nitrification, and sediment oxygen demand. A eutrophication model defines the interactions of algae and nutrients. Using the results of the in-stream model, point source loads of nutrients and dissolved oxygen are simulated at the confluence of the mainstem of the Housatonic River with the tributary reaches.

HSPF-AQUATOX

Point source loads of inorganic nutrients and dissolved oxygen, contributed by tributary inflows and wastewater dischargers, are input at the upstream boundary of each AQUATOX reach. Nonpoint source loads, generated from the surface and subsurface runoff components of HSPF, are aggregated over each HSPF reach and input at the upstream boundary of each AQUATOX reach. The sum of point and nonpoint source loads of dissolved oxygen and nutrients generated by HSPF are numerically integrated for input as the upstream boundary to AQUATOX as time series of daily loads as follows:

Dissolved oxygen……………………………………………………………….(g day^{-1})
Ammonia-N……………………………………………………………………..(g day^{-1})
Nitrite-N + Nitrate-N…………………………………………………………….(g day^{-1})
Orthophosphate-P……………………………………………………………….(g day^{-1})

4.4.2.3 Solids, BOD, and Organic Matter

Figure 4-14 illustrates the linkage of nonpoint and point source loads of solids, BOD, and organic carbon generated by HSPF as input to EFDC and AQUATOX. Suspended solids are provided by HSPF to EFDC while organic carbon and BOD are provided by HSPF to AQUATOX. This section describes the methodology that will be used to link suspended solids, bedload solids, BOD and organic carbon provided by HSPF and EFDC, and the transformation of these loads to inorganic solids and organic matter needed to maintain a correct mass balance for input to AQUATOX.

HSPF

HSPF generates TSS, BOD, and TOC with the simulated loads calibrated to observed TSS, BOD, and TOC data collected in the tributaries and at mainstem stations of the Housatonic River. TSS loads generated by HSPF account for both organic and inorganic components of suspended solids. BOD and TOC loads generated by HSPF account for both dissolved and particulate forms of organic carbon. HSPF generates nonpoint source loads delivered to the edge of a stream as subsurface inputs of BOD and surface runoff of TSS and BOD over the incremental drainage area between tributary reaches. Using cohesive and noncohesive size

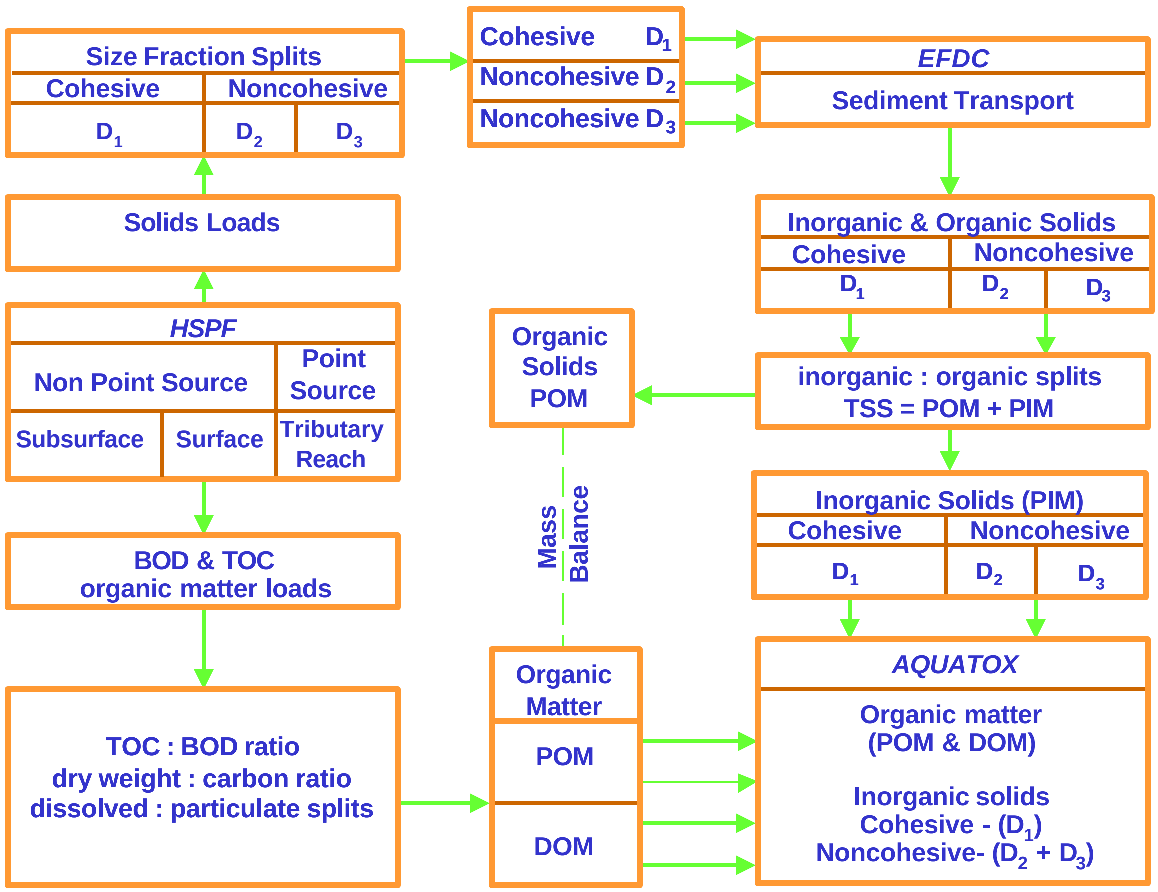

Figure 4-14 Model Linkage Within the Modeling Framework for TSS, BOD, and Organic Matter

fraction splits for TSS and TOC:BOD ratios to transform nonpoint source loads of TSS and BOD for input to tributary reaches, HSPF generates point source loads of cohesive (silts and clays) and noncohesive (sands) solids, BOD, and TOC at the confluence of the mainstem of the Housatonic River with the tributary reaches. A one-dimensional water quality model is used for instream advective routing with kinetic sources and sinks simulated in the mainstem and tributary reaches.

HSPF-EFDC

In EFDC, inorganic solids are represented as suspended solids and bedload solids using three size classes: (1) cohesive (< 63 microns); (2) fine to medium noncohesive (63 to 250 microns); and (3) coarse noncohesive (>250 microns). Using site-specific grain size distribution data to define spatial and seasonally varying size fraction splits for TSS, nonpoint source surface runoff loads of TSS from HSPF are split to provide input time series to EFDC as three classes of cohesive and noncohesive solids. Nonpoint source loads of TSS generated by HSPF are distributed to each EFDC grid cell in proportion to the length of the grid cell and the length of the HSPF mainstem reach. Point source loads of TSS contributed by tributary inflows and wastewater discharges are input to specific EFDC grid cells to correspond to the spatial location of the tributary or wastewater discharge inflows. Hourly time series of suspended solids loading data provided by HSPF for input to EFDC are linearly interpolated in EFDC to match the high-frequency time step (< hour) needed for the hydrodynamic and sediment transport model. For both nonpoint and point sources, TSS loads are input to EFDC grid cells as time series data sets of boundary inflows (cubic meters per second) and TSS concentrations (mg/L) for the three size classes of solids.

Suspended solids are input to EFDC at a grid cell as hourly time series of boundary inflows and suspended solids concentration as follows:

Boundary inflow…………………………………………………………………(m^3 sec^{-1})
TSS#1 (cohesive, <63 microns)……………………………………………………….(mg/L)
TSS#2 (noncohesive, 63-250 microns)………………………………………………..(mg/L)
TSS#3 (noncohesive, >250 microns)………………………………………………….(mg/L)

EFDC-AQUATOX

EFDC generates a fine grid distribution of cohesive and noncohesive solids driven by the simulation of suspended load and bedload processes. Cohesive and noncohesive solids mass fluxes ([flow] x [concentration]) are summed over the EFDC grid cells across the upstream boundary and the channel/floodplain boundary of the matching AQUATOX reach. Deposition and resuspension mass fluxes ([velocity] x [concentration]) for solids are summed over the EFDC grid cells that correspond to each AQUATOX reach. The upstream mass flux of solids, floodplain/channel solids flux (to/from), deposition flux, and resuspension flux of solids are numerically integrated over a 24-hour period for input to AQUATOX as daily time series.

TSS represented in both HSPF and EFDC include both particulate organic (POM) and particulate inorganic (PIM) components of matter. Since POM is provided to AQUATOX from HSPF via transformations of BOD and TOC, the organic matter fraction of TSS (i.e., POM) represented in

EFDC must be excluded from the linkage to AQUATOX. As shown in Figure 4-14 with a dashed line, the mass flux of POM subtracted from the TSS flux simulated in EFDC must balance the mass load of POM provided by HSPF to AQUATOX. Site-specific field data are used to define spatial and seasonal splits for the organic fraction of TSS as the ratio of TOC:TSS and the ratio of dry weight:carbon (DW:C) to estimate the POM accounted for as TSS in EFDC (see Eq. 4-3). To maintain a correct mass balance of inorganic (PIM) and organic (POM) matter provided by HSPF and EFDC to AQUATOX, the organic matter component (POM) (see Eq. 4-5) must be subtracted as shown in Eq. 4-6 from the cohesive and noncohesive solids fluxes (Eq. 4-4) provided by EFDC to AQUATOX:

$$\text{TSS} = \text{POM} + \text{PIM} \quad \text{Eq. (4-3)}$$

$$\text{PIM} = \text{noncohesive (sands)} + \text{cohesive (silts and clays)} \quad \text{Eq. (4-4)}$$

$$\text{POM} = \text{TSS} * (\text{TOC:TSS}) * (\text{DW:C}) \quad \text{Eq. (4-5)}$$

$$\text{PIM} = \text{TSS} - \text{POM} = \text{TSS} * [1 - (\text{TOC:TSS}) * (\text{DW:C})] \quad \text{Eq. (4-6)}$$

The inorganic matter (PIM) component of suspended solids generated in EFDC is provided as a time series to AQUATOX as horizontal fluxes of cohesive and noncohesive inorganic solids at the upstream boundary, the channel/floodplain boundary, and vertical fluxes at the bed-water interface representing deposition and resuspension. Using seasonal and spatially varying estimates of TOC:TSS in the water column of the Housatonic River and tributaries, horizontal fluxes of inorganic solids across the upstream and river/floodplain boundaries for the cohesive and two noncohesive size classes are determined using Eq. 4-6. Solids deposition fluxes provided to AQUATOX are also transformed using seasonal and spatially varying water column estimates of TOC:TSS. Solids resuspension fluxes provided from EFDC to AQUATOX are transformed using seasonally and spatially varying sediment bed estimates of TOC:TSS. Horizontal fluxes at the upstream boundary and the channel/floodplain boundary and vertical fluxes of deposition and resuspension are provided to AQUATOX as time series data sets for cohesive and noncohesive solids with units of grams per day.

In the river channel, backwater areas of the river, and Woods Pond, net sediment accumulation is accounted for by external watershed loading of inorganic solids and particulate organic matter and internally produced biogenic organic matter. In contrast to EFDC, in which internal biological production of organic matter is not represented in the sediment transport model, AQUATOX does account for internal biological production of particulate organic matter and subsequent net deposition between the water column and the sediment bed. Deposition and resuspension processes of POM are parameterized in AQUATOX by assuming that the behavior of cohesive solids subject to deposition and resuspension in EFDC can be used to infer equivalent deposition and resuspension velocities for POM that would also be subject to the same physical processes as cohesive solids. Deposition and resuspension fluxes simulated in EFDC for the cohesive size class of solids are aggregated over the grid cells corresponding to each AQUATOX reach to compute equivalent velocities to simulate deposition and resuspension fluxes of POM in AQUATOX as:

TSS#1 (cohesive, deposition velocity)……………………………………………….(m day^{-1})
TSS#1 (cohesive, resuspension velocity)…………………………………………….(m day^{-1})

EFDC provides AQUATOX with the total solids sum of suspended and bedload particulate inorganic solids (PIM) (computed from Eq. 4-4) as daily time series to define upstream boundary conditions (BC) input data as:

Solids PIM#1 BC (cohesive, <63 microns)……………………………………………(g day^{-1})
Solids PIM#2 BC (noncohesive, 63-250 microns)…………………………………….(g day^{-1})
Solids PIM#3 BC (noncohesive, >250 microns)………………………………………(g day^{-1})

EFDC provides AQUATOX with suspended loads of particulate inorganic solids (PIM) (computed from Eq. 4-6) as daily time series to define the export/import (E/I) of solids to/from the river channel and floodplain (R/FP) as:

Suspended PIM#1 R/FP E/I (cohesive, <63 microns)……………………………….(g day^{-1})
Suspended PIM#2 R/FP E/I (noncohesive, 63-250 microns)………………………..(g day^{-1})
Suspended PIM#3 R/FP E/I (noncohesive, >250 microns)………………………….(g day^{-1})

Because the physical domain of AQUATOX does not include the floodplain, the total PCB load provided by HSPF to AQUATOX must be adjusted internally within AQUATOX to account for the mass flux export(loss)/import(gain) of PCBs sorbed onto solids between the river channel and floodplain. The mass flux of solids exchanged between the river channel and the floodplain provided by EFDC is coupled with the internally generated concentration of sorbed and dissolved PCBs simulated in AQUATOX to specify the mass flux exchange of sorbed PCBs from the river channel to the floodplain. For floodplain resuspension, which is considered a very rare occurrence, a zero flux condition of PCBs resuspended from the floodplain to the river is assumed.

EFDC provides AQUATOX with the mass fluxes of suspended particulate inorganic solids (PIM) (computed from Eq. 4-6) as daily time series to define deposition and resuspension of solids as:

Suspended PIM#1 Deposition (cohesive, <63 microns)………………………………(g day^{-1})
Suspended PIM#2 Deposition (noncohesive, 63-250 microns)……………………….(g day^{-1})
Suspended PIM#3 Deposition (noncohesive, >250 microns)…………………………(g day^{-1})

Suspended PIM#1 Resuspension (cohesive, <63 microns)……………………………(g day^{-1})
Suspended PIM#2 Resuspension (noncohesive, 63-250 microns)…………………….(g day^{-1})
Suspended PIM#3 Resuspension (noncohesive, >250 microns)………………………(g day^{-1})

HSPF-AQUATOX

Using site-specific data to characterize spatial and seasonally varying ratios for TOC:BOD and dissolved (DOC:TOC) and particulate (POC:TOC) fractions of TOC, nonpoint source subsurface and surface runoff loads of BOD are transformed to provide time series input to AQUATOX as dissolved (DOC) and particulate (POC) organic carbon. The dissolved and particulate components of TOC are further split with a dry weight to carbon (DW:C) conversion of organic carbon to organic matter (as dry weight) for input to AQUATOX. The arithmetic definitions and procedures for linkage of HSPF output as input to AQUATOX are given by the following set of equations:

BOD = dissolved BOD + particulate BOD…………………………………Eq. (4-7)
TOC = DOC + POC………………………………………………………..Eq. (4-8)

Subsurface and surface runoff BOD loads generated by HSPF are transformed to TOC as follows:

TOC = BOD * (TOC:BOD)…………………………………………………Eq. (4-9)

Using a DW:C ratio, TOC generated by HSPF in the tributaries, and the subsurface and surface runoff load of BOD transformed to TOC using Eq. 4-9 is split into dissolved and particulate fractions of organic matter (as dry weight) as follows:

DOM = TOC * (DOC:TOC) * (DW:C)……………………………………Eq. (4-10)
POM = TOC * (POC:TOC) * (DW:C)……………………………………Eq. (4-11)

Nonpoint and point source loads of organic matter accounted for by subsurface and surface runoff, tributary inflows, and wastewater discharges are input at the upstream boundary of each AQUATOX reach. Using Eq. 4-9 through Eq. 4-11, HSPF provides AQUATOX with the sum of point and nonpoint source loads of dissolved (DOM) and particulate (POM) organic matter as daily time series to define the following upstream boundary loads :

DOM……………………………………………………………………….(g day^{-1})
POM……………………………………………………………………….(g day^{-1})

4.4.2.4 PCBs

Figure 4-15 illustrates the linkage of loads of total PCBs generated by HSPF as input to EFDC and AQUATOX. Total PCBs are provided by HSPF to EFDC while total PCBs provided by HSPF are split as homologs and selected congeners for input to AQUATOX as described below. EFDC will simulate total PCBs as an abiotic constituent with the primary process being adsorption and desorption of total PCBs with solids. AQUATOX will simulate abiotic processes for PCBs (e.g., adsorption and desorption), biotransformation, and bioaccumulation of PCBs within the Housatonic River system. EFDC will track the mass balance of the deposition of sorbed PCBs onto the floodplain. In addition, on a much finer spatial scale of resolution than that for the coarse spatial scale used in AQUATOX, the simulation of total PCBs in EFDC will allow for the high-resolution spatial distribution of PCBs.

The following sections describe the methodology that will be used to link total PCB concentrations provided by HSPF to EFDC and by HSPF to AQUATOX. These sections also describe the transformation of total PCB loads to homologs and selected congeners as needed to maintain a correct mass balance for input of PCBs to AQUATOX.

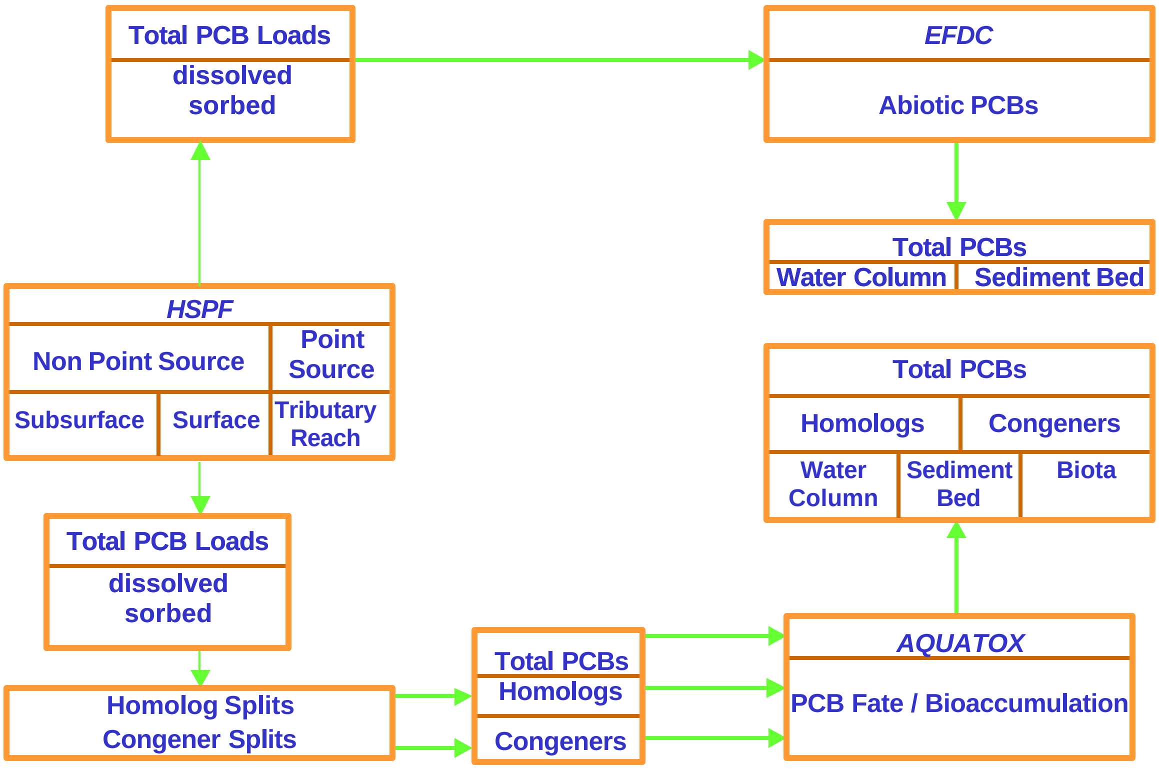

Figure 4-15 Model Linkage Within the Modeling Framework for PCBs

HSPF

HSPF generates total PCB loading from surface runoff of dissolved and sorbed PCBs and subsurface inflow of dissolved PCBs over the drainage area of each HSPF catchment subbasin, and from instream tributary reaches or boundary conditions, with total PCBs split into three components: (1) dissolved PCBs, (2) PCBs sorbed on cohesive solids, and (3) PCBs sorbed on noncohesive solids. Dissolved and sorbed components of PCBs are simulated internally in HSPF for advective routing using partition coefficients for noncohesive and cohesive solids within tributary reaches. Simulated PCB loads are calibrated to observed total PCB data in tributaries and the mainstem stations of the Housatonic River. Total PCBs generated by HSPF are considered to account for both the dissolved and sorbed components.

HSPF-EFDC

Loadings of PCBs from tributary inflows are input to specific EFDC grid cells corresponding to the spatial locations of the source inflows. Hourly time series of PCB loading data provided by HSPF for input to EFDC are linearly interpolated in EFDC to match the high-frequency time step (~minutes) needed for the hydrodynamic model. Total PCBs are input to EFDC at a grid cell as hourly time series of boundary inflows and concentration as follows:

Boundary inflow…………………………………………………………………(m^3 sec^{-1})
Total PCBs……………………………………………………………………..(µg/L)

The PCB transport and abiotic fate submodel in EFDC generates a fine grid distribution of total PCBs for the water column and the sediment bed, including the distribution of sorbed PCBs in the floodplain that results from overbank flow. Total PCBs are partitioned in the model as dissolved and sorbed fractions. PCB partition coefficients assigned to cohesive and noncohesive size classes of solids are used in EFDC to account for the abiotic fate of total PCBs. Observed total PCBs measurements in the water column and sediment bed are compared to simulated total PCBs for calibration and validation of the abiotic PCB transport and fate model of EFDC.

HSPF-AQUATOX

Loadings of total PCBs from tributary inflows are input at the upstream boundary of an AQUATOX reach. The watershed model (HSPF) simulates loading of total abiotic PCBs as dissolved and sorbed forms of PCBs.

AQUATOX simulates the bioaccumulation of three forms of PCBs: (1) total PCBs; (2) PCB homologs; and (3) selected congeners. The total PCB loads simulated in HSPF, adjusted to account for the sorbed PCB exchange between the river channel and floodplain, must be transformed to define multiple homolog and selected congener loads of PCBs for input to AQUATOX. Using splits of total PCBs to define multiple homologs and selected congeners, total PCB loads are defined for input to AQUATOX using three forms of PCBs as: (1) total PCBs; (2) homologs; and (3) selected congeners of PCBs as follows:

Total PCBs……………………………………………………………………(g day^{-1})
PCB homologs……………………………………………………...…………(g day^{-1})
Selected PCB congener(s)……………………………………………………(g day^{-1})

PCB partition coefficients assigned to dissolved and particulate organic matter are used in AQUATOX to account for fate and bioaccumulation of total PCBs, multiple homologs, and selected congeners of PCBs. Observed PCB measurements in the water column (dissolved and sorbed), sediment bed, and biota are compared to simulated PCBs in these three compartments for calibration and validation of the PCB bioaccumulation model of AQUATOX.